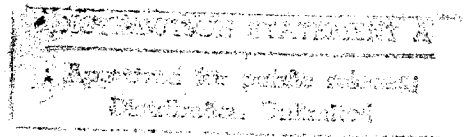


X-18020

Subject Category: PHYSICS AND MATHEMATICS

NEUTRON FLUX DISTRIBUTIONS IN MULTIPLE REGION REACTORS

100-443886-100



19950811 121

DTIC QUALITY INSPECTED 5

Date Declassified: December 6, 1951.

This report was prepared as a scientific account of Government-sponsored work and is made available without review or examination by the Government. Neither the United States, nor the Commission, nor any person acting on behalf of the Commission makes any warranty or representation, express or implied, with respect to the accuracy, completeness, or usefulness of the information contained in this report, or that the use of any information, apparatus, method, or process disclosed in this report may not infringe privately owned rights. The Commission assumes no liability with respect to the use of, or for damages resulting with respect to the use of any information, apparatus, method, or process disclosed in this report.

This report has been reproduced directly from the best available copy.

Issuance of this document does not constitute authority for declassification of classified material of the same or similar content and title by the same authors.

Printed in USA, Price 40 cents. Available from the Office of Technical Services, Department of Commerce, Washington 25, D. C.

NEUTRON FLUX DISTRIBUTIONS IN MULTIPLE REGION REACTORS

Sylvan Wallach

December 1951

Accession For	
THIS GRANT	<input checked="" type="checkbox"/>
THIS TASK	<input type="checkbox"/>
Unannounced	<input type="checkbox"/>
Justification	
By	
Discipline	
Availability	
Work Center	
Dist	Spec
A-1	

Naval Reactor Program
Contract AT-11-1-GEN-14

WESTINGHOUSE ELECTRIC CORPORATION
ATOMIC POWER DIVISION
P. O. Box 1468 Bettis Field
Pittsburgh 30 Pennsylvania

TABLE OF CONTENTS

ABSTRACT	5
SYMBOLS	6
NEUTRON FLUX DISTRIBUTIONS IN MULTIPLE REGION REACTORS	
Introduction	7
I. <u>The Integral Equation for Diffusing Media</u>	10
1. The Two Group Diffusion Equations	10
2. The Modified Two Group Integral Equation	12
3. Formal Solution by Iteration	15
4. Convex Regions	18
5. The Slab Water Hole in an Infinite Reactor	25
6. The Cylindrical Water Hole in an Infinite Reactor	29
7. Non-Convex Regions	31
8. The Cross Shaped Water Hole	33
9. Appendix to Part I	37
II. <u>The Method of Superposition</u>	40
1. Superposition by Addition	42
2. Superposition by Multiplication	51
3. Combined Superposition	57
4. Conclusion	58
III. <u>Other Applications</u>	60
1. Control Rods	60
2. Superposition of Control Rods	62
3. Generalizations	63

NEUTRON FLUX DISTRIBUTIONS IN MULTIPLE REGION REACTORS

- ABSTRACT -

In this report the problem is considered of determining neutron flux distributions in reactors consisting of discrete regions of substantially different nuclear properties.

Starting with these equations the problem is considered of determining the flux in one of the energy groups given the spatial flux distribution of the next higher energy group. The problem is handled by converting the differential equation with source term to an integral equation; under appropriate conditions the integral equation may be solved by a numerical iterative procedure. The conditions under which this may be done are discussed and formulas are developed for placing bounds on the errors. In addition the technique of obtaining flux distributions in complicated configurations by additive and multiplicative superposition of flux distributions of simpler configurations is considered. Expressions are derived for estimating the errors made in using these methods. A number of simple examples are presented.

SYMBOLS

A, B	see page 16
D_i	neutron diffusion constant in i 'th medium
D_s	thermal neutron group diffusion constant
D_f	fast neutron group diffusion constant
G	Green's function
R_i	the i 'th region
S_i	the surface of the i 'th region
k	material multiplication constant
p	resonance escape probability
q_i	source strength of neutrons in the i 'th region
$\underline{r}, \underline{r}'$	position vectors
α, β, γ	see page 18
ϵ_n	error in the n 'th iterate
κ_i	$(\Sigma_i/D_i)^{1/2}$
Σ	neutron absorption cross section
Σ_s	thermal neutron group absorption cross section
Σ_f	fast neutron group absorption cross section
φ	neutron flux
φ_s	thermal neutron flux
φ_f	fast neutron flux
∇	gradient operator
$\partial/\partial n$	derivative in the direction of the normal

NEUTRON FLUX DISTRIBUTIONS IN MULTIPLE REGION REACTORS

Sylvan Wallach

INTRODUCTION

The studies reported in this paper were carried out to develop methods for determining the flux distributions in reactors made up of discrete regions of substantially different nuclear properties.

A procedure for calculating the flux distribution by an iterative technique is presented here as well as certain analytical results pertaining to the general problem. This work was carried out at the Westinghouse Atomic Power Division under Atomic Energy Commission Contract AT-11-1-GEN-14.

The problem of determining the thermal neutron flux for a reactor having discrete regions has been considered within the framework of multi-group diffusion theory. A two-group model is used.

A very considerable simplification of the problem can be made by assuming in the two-group case that the fast flux spatial distribution is known or may be satisfactorily approximated. For the multi-group case a similar remark applies to the flux in the group next higher in energy than the one under consideration. From a mathematical point of view the problem then becomes one of finding appropriate solutions to the Helmholtz equation with sources in multiple regions with boundary conditions given for the function and possibly its gradient.

The problem outlined may be attacked by direct numerical solution of the differential equation with boundary conditions. This is the technique which has been used successfully by Garabedian and Schiff.^{*} They have applied the relaxation method of Southwell to determine the flux distributions at and about cross shaped water channels. Another approach, the one developed in this report, is to convert the differential equation and boundary conditions to an integral equation. The integral equation lends itself well both to analysis and to solution by numerical procedures. No comparison of the two techniques, insofar as numerical solution is involved, has been attempted. It is likely that both methods have their respective advantages which may be significant in specific situations. The integral equation approach is, as will be seen,

^{*} H. L. Garabedian and R. R. Schiff,
WAPD-RM-89.

amenable to analysis and permits bounds to be set on the errors involved in the numerical solution. Further it appears that fairly good results can be obtained with it starting with poor initial approximations

Part I of this report is concerned with the derivation of the integral equation and a discussion of its form. An iterative procedure for solution of the equation is developed and the conditions under which the iterative procedure converges is studied. It is shown

that the iterative procedure converges for a convex water hole. Bounds for the errors in the iterates are developed under these convergent conditions. It is also shown that the iteration will fail to converge under certain circumstances. Simple examples of a slab water hole and a cylindrical water hole in an infinite reactor are solved to illustrate the technique. Finally a cross water hole is considered to illustrate the procedure for a non-convex region.

Part II consists of a discussion of the technique of additive superposition to obtain flux distributions by addition of the distributions for simple regions and the technique of multiplicative superposition to obtain flux distributions for finite reactors. As an example of additive superposition a cross water channel is solved by superposing cylindrical water holes. Expressions for the errors introduced in superposition are developed for both additive and multiplicative superposition. Several additional examples in slab geometry are included to illustrate the methods.

I. THE INTEGRAL EQUATION FOR DIFFUSING MEDIA

This part of the report is devoted to the derivation of the integral equation, a description of its use, and its application to some simple problems. It will be shown how bounds for the flux can be estimated and sufficient conditions for the convergence of successive approximations will be derived.

1. The Two Group Diffusion Equations

The steady state two group diffusion equations are

$$(I.1) \quad \nabla D_s \nabla \phi_s - \Sigma_s \phi_s + p \Sigma_f \phi_f = 0$$

$$(I.2) \quad \nabla D_f \nabla \phi_f - \Sigma_f \phi_f + \frac{k}{p} \Sigma_s \phi_s = 0 .$$

Suppose we are interested not in criticality, but only in the thermal neutron flux distribution. Then, rather than attempt to solve a complicated characteristic value problem, it is frequently sufficient to guess at the form of ϕ_f and to solve (I.1) for ϕ_s . The slow flux thus obtained is often a very good approximation to the correct flux.* Instead of (I.1) and (I.2), let us therefore consider for the present

$$(I.3) \quad \nabla D \nabla \phi - \Sigma \phi + q = 0 ,$$

where we are now interested only in the thermal neutron flux and $q = p \Sigma_f \phi_f$ is the source term for thermal neutrons. Of course ϕ can be any neutron energy group of interest and q the appropriate source term. It is equation (I.3)

* If desired, the assumed values for ϕ_f can be checked by putting the calculated ϕ_s in equation (I.2) and solving for ϕ_f . If the iteration is continued, and if the solutions obtained are suitably normalized, the iterations can be expected to converge to the fundamental modes of the fast and thermal fluxes.

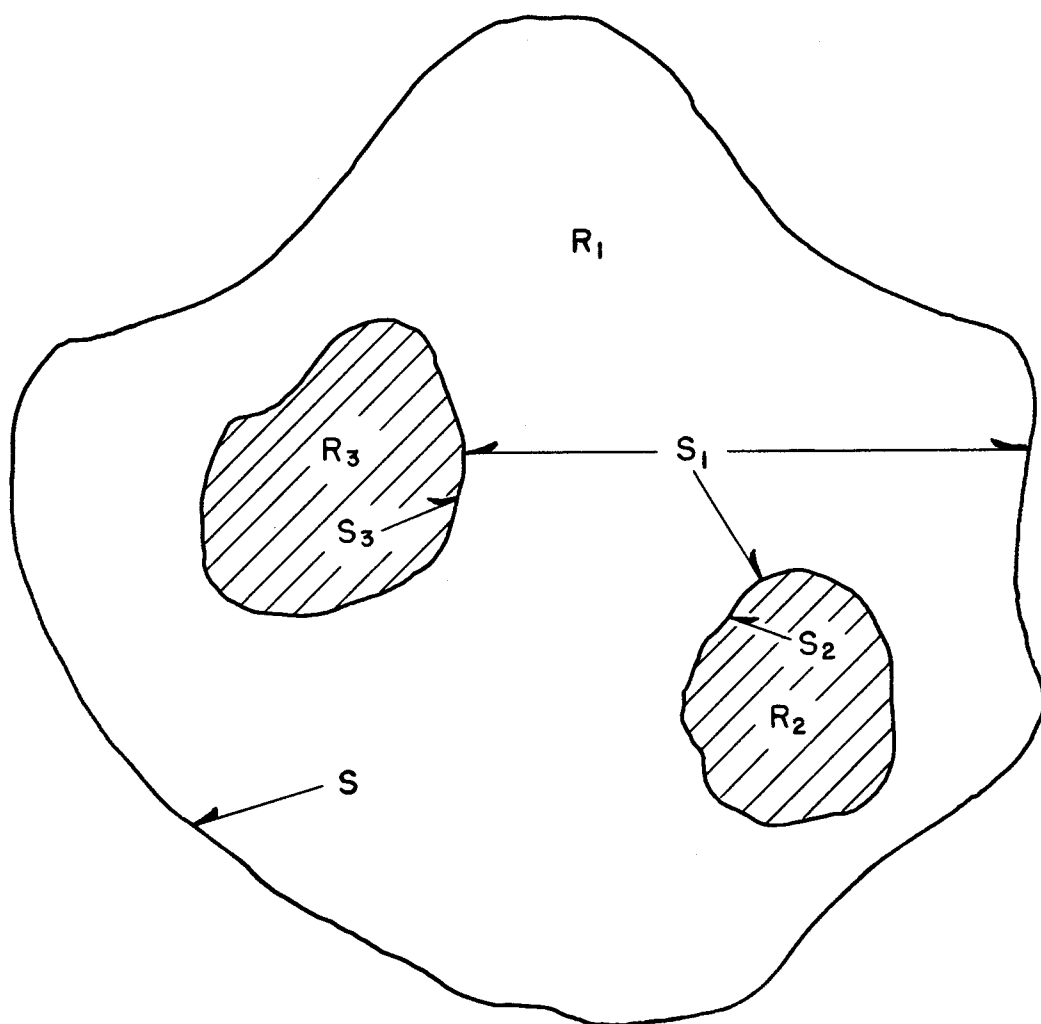


FIGURE I

REACTOR CONSISTING OF 3 HOMOGENEOUS MEDIA

to which Garabedian and Schiff have applied the relaxation technique and which we shall now convert to an integral equation. Frequently equation (I.3) is referred to as a one group theory although it is much more closely related to two group diffusion theory than to the one group theory from which is derived the equation $\nabla D \nabla \phi + (k-1) \Sigma \phi = 0$. It would be apt to say that (I.3) is based on a modified two group theory.

2. The Modified Two Group Integral Equation

In this section the integral equation defining the thermal flux distribution in a region consisting of three homogeneous diffusing media will be derived from equation (I.3). The usual boundary conditions, i.e., continuity of flux and of current at interfaces, will apply. On finite boundaries $\phi = 0$; if the medium extends to infinity it is required that ϕ remain bounded. The latter requirement ensures the vanishing of a surface integral, $\int \phi \frac{\partial G}{\partial n}$, where G is a Green's function to be defined below. Consider some arrangement of the media such as is shown in Figure 1.

Let us rewrite equation (I.3)

$$(I.4) \quad \nabla D \nabla \phi - \Sigma_1 \phi = (\Sigma - \Sigma_1) \phi - q \quad ,$$

and consider also

$$(I.5) \quad D_1 \nabla^2 G - \Sigma_1 G = 0 \quad .$$

The solution G of (I.5) is the Green's function appropriate to the total volume under consideration, and the boundary conditions. It is the flux distribution created by a point source of neutrons. If the region is finite, then G vanishes on the outermost boundary, S ; if the region extends to infinity, then G tends to zero at infinity. More precisely, in the two dimensional case, $G(\underline{r}, \underline{r}^0)$ is the solution of (I.5) which vanishes on the boundary, S , which has a

logarithmic singularity at \underline{r} and which is normalized so that

$$\int_{R_{1+2+3}} G = \frac{D_1}{\Sigma_1} \int \underline{1} + \int_S \frac{\partial G}{\partial n} \underline{1} .$$

If the medium R_1 extends to infinity in all directions then $G = K_0(\kappa_1 |\underline{r} - \underline{r}'|) / 2\pi$, where K_0 is the zeroth order Bessel's function of the second kind with imaginary argument.

Let us call region R_1 the external region and regions R_2 and R_3 internal regions. Let the point of interest be an internal point, say at \underline{r} in R_3 . Multiply equation (I.4) by G , equation (I.5) by φ , subtract, and integrate over all three regions with the exception of a sphere, Σ , of radius ϵ around the point \underline{r} . Transform the integrals by Green's theorem and let $\epsilon \rightarrow 0$. Observe that

$$\lim_{\epsilon \rightarrow 0} \int_{S_\Sigma} G \frac{\partial \varphi}{\partial n} = 0 , \quad \lim_{\epsilon \rightarrow 0} \int_{S_\Sigma} \varphi \frac{\partial G}{\partial n} = \varphi .$$

There results, in view of the boundary conditions and the continuity of G and its gradient,

$$\begin{aligned} \text{(I.6)} \quad -D_1 \varphi + (D_1 - D_2) \int_{R_2} \nabla \varphi \cdot \nabla G + (D_1 - D_3) \lim_{\epsilon \rightarrow 0} \int_{R_3 - \Sigma} \nabla \varphi \cdot \nabla G \\ = \int_{R_{1+2+3}} G \int (\Sigma - \Sigma_1) \varphi - q \end{aligned}$$

Now

$$\begin{aligned} \int_{R_2} \nabla \varphi \cdot \nabla G &= \int_{S_2} \varphi \frac{\partial G}{\partial n} - \int_{R_2} \varphi \nabla^2 G \\ &= \int_{S_2} \varphi \frac{\partial G}{\partial n} - \int_{R_2} \varphi \frac{\Sigma_1}{D_1} G . \end{aligned}$$

Also

$$\lim_{\epsilon \rightarrow 0} \int_{R_3 - \Sigma} \nabla \varphi \cdot \nabla G = \int_{S_3} \varphi \frac{\partial G}{\partial n} + \varphi - \int_{R_3} \varphi \frac{\Sigma_1}{D_1} G \quad .$$

Substituting in (I.6) and making some rearrangements, we obtain

$$\begin{aligned} (I.7) \quad D_3 \varphi = & (D_1 - D_2) \int_{S_2} \varphi \frac{\partial G}{\partial n} + (D_1 - D_3) \int_{S_3} \varphi \frac{\partial G}{\partial n} \\ & + (\kappa_1^2 - \kappa_2^2) D_2 \int_{R_2} G \varphi + (\kappa_1^2 - \kappa_3^2) D_3 \int_{R_3} G \varphi \\ & + \int_{R_{1+2+3}} q_1 G + \int_{R_2} (q_2 - q_1) G + \int_{R_3} (q_3 - q_1) G \quad . \end{aligned}$$

It is evident from the symmetry in the right hand side of (I.7) that exactly the same expression will be obtained for $D_2 \varphi$ if the point \underline{r} is in region R_2 . It is also clear how additional regions can be included. Perhaps not so obvious is the fact that for points in region R_1 , $D_1 \varphi$ also is given by the right side of (I.7). It must be remembered, however, that the singularity of G is at the point \underline{r} of interest, and that the contributions of the surface integrals undergo discontinuities as the point \underline{r} crosses an interface between media. Thus the content, if not the form, of the right hand side of (I.7) is different in the three cases.

Equation (I.7) is an inhomogeneous linear integral equation for the flux φ . It should be noted that the integrals containing φ involve only the internal regions R_2 and R_3 . Thus the integral equation can be solved for the flux in regions R_2 and R_3 without any consideration of the flux in R_1 . After the flux in R_2 and R_3 has been determined, the flux in region R_1 can be obtained by integration. This fact is important in solving (I.7) by iteration.

It is necessary only to assume trial values for the flux and to iterate in regions R_2 and R_3 in order to determine the flux there.

In solving (I.7) by iteration the flux on the boundaries of regions R_2 and R_3 can be found in two ways, according as the boundary points are considered internal points or external points. In some cases the flux at external points, obtained by one iteration, is very much less sensitive to the starting values than is the internal flux. Hence it may sometimes be advantageous to estimate starting values for the iteration in regions R_2 and R_3 , iterate once to obtain improved values on the boundaries of R_2 and R_3 , and then to make new estimates of the flux in R_2 and R_3 from these boundary values.

The integral equation (I.7) divides the contributions to ϕ neatly into three parts--the first part caused by the differences in the diffusion constants, the second part caused by the differences in the κ 's, and the third part caused by the differences in the source terms. This fact can be very useful. In a given problem it will be clear how to alter the values of the constants so as to obtain simpler integral equations whose solutions majorize and minorize the flux sought. It is particularly advantageous, from the point of view of computation, to eliminate the surface integrals. The extreme example of this device is the majorant provided by the maximum value of q_i/\sum_i and the minorant provided by the minimum value of q_i/\sum_i , i.e. the largest and smallest asymptotic values of the fluxes.

3. Formal Solution by Iteration

In this section the solution of the integral equation (I.7) by the method of successive approximations will be discussed in a purely formal manner. Questions of convergence are deferred to sections 4 and 7. We consider only the physically interesting case in which D_i , \sum_i , q_i are non-negative and all $q_i \neq 0$, and we take it for granted that the integral equation then has a unique solution which is positive everywhere.

For simplicity write the integral equation (I.7) in the form

$$(I.8) \quad \varphi = A\varphi + B, \quad ,$$

where A is a linear integral operator and B is a known function. Let φ be the solution of (I.8) and let $\varphi_0 = \varphi + \epsilon_0$ be a zeroth approximation. Neither the flux φ nor the error ϵ_0 is known, only their sum φ_0 is given. Then the successive approximations are defined by

$$(I.9) \quad \varphi_n = A\varphi_{n-1} + B.$$

The error ϵ_0 is itself the solution of an integral equation like (I.8), for we have

$$(I.10) \quad \epsilon_0 = A\epsilon_0 + \varphi_0 - \varphi_1.$$

Bounds for the error ϵ_0 can be estimated from (I.10).

The errors in the successive approximations are obtained as follows:

$$(I.11) \quad \begin{aligned} \epsilon_1 &= \varphi_1 - \varphi = A(\varphi_0 - \varphi) = A\epsilon_0 \\ \epsilon_2 &= A\epsilon_1 = A^2\epsilon_0 \\ &\vdots \\ \epsilon_n &= A^n\epsilon_0 \\ &\vdots \end{aligned}$$

Hence the error $\epsilon_n \rightarrow 0$ if and only if $A^n\epsilon_0 \rightarrow 0$. The important fact is that if it is possible to derive an estimate $|\epsilon_n| \leq \eta |\epsilon_{n-1}|$, $0 < \eta < 1$, from the equality $\epsilon_n = A\epsilon_{n-1}$, then it can be asserted that the error is reduced by at least the fraction $1-\eta$ at each iteration. Together with an estimate of

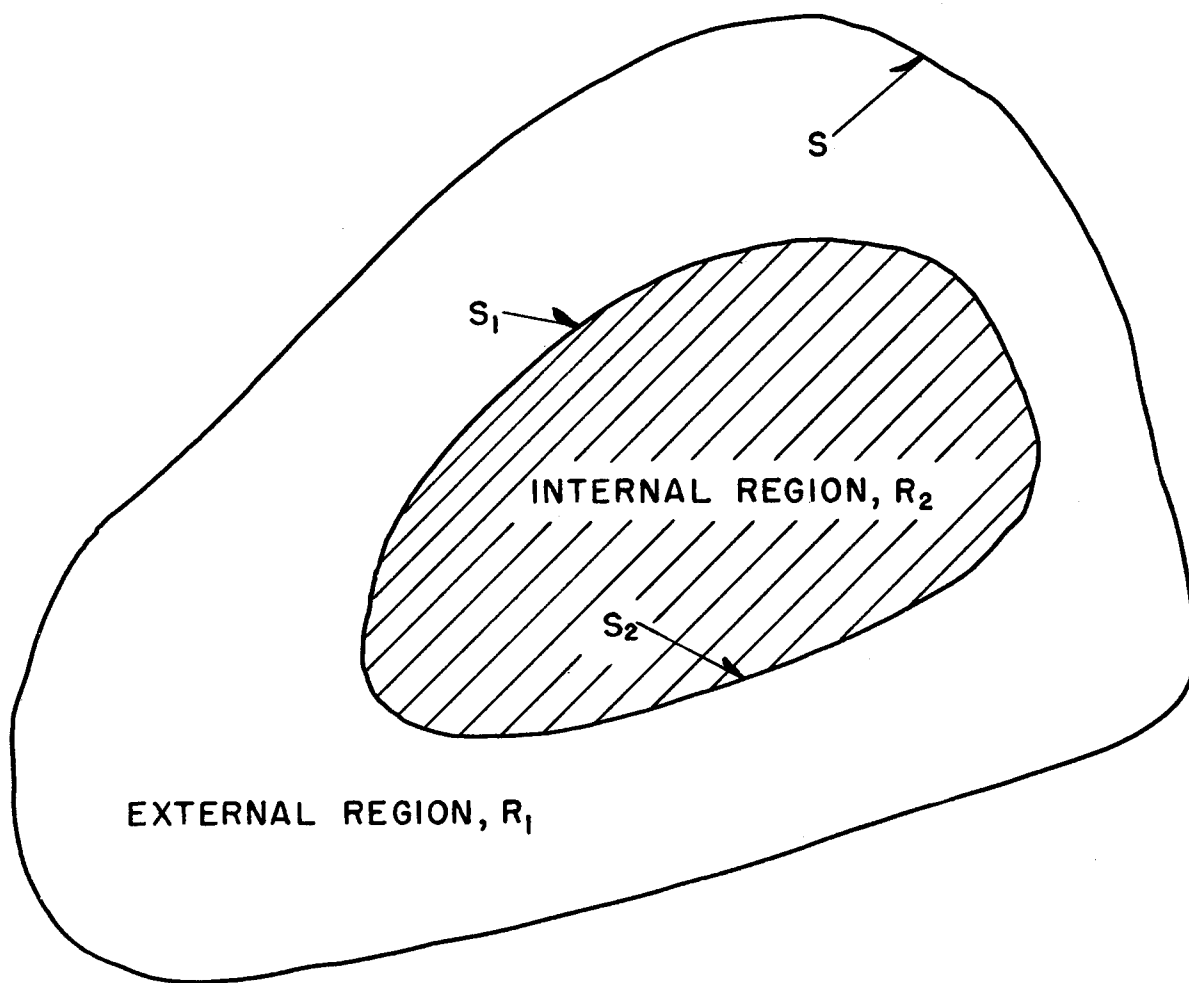


FIGURE 2
SINGLE CONVEX INTERNAL REGION

ϵ_0 , one is then in a position to determine a bound for the error in any iterate. Clearly the convergence of the successive approximations to φ is equivalent to $\epsilon_n \rightarrow 0$.

4. Convex Regions

This section, and section 7 below, are concerned with the problem of convergence of the successive approximations defined by (I.9). For a single convex internal region the question of convergence is answered by the theorem on page 22. The present section contains the proof of this theorem, as well as derivations of inequalities giving bounds for the flux and the errors. Non-convex regions, for which less is known, are discussed in section 7. By way of examples, the flux distribution in a slab water hole is calculated in section 5, and in a cylindrical water hole in section 6.

A convex region is defined by the property that every chord intersects the surface at most twice.

Let R_2 , Figure 2, be convex. The flux in R_2 is the solution of

$$(1.12) \quad D_2 \varphi = (D_1 - D_2) \int_{S_2} \varphi \frac{\partial G}{\partial n} + (\kappa_1^2 - \kappa_2^2) D_2 \int_{R_2} \varphi G + \int_{R_{1+2}} q_1 G + \int_{R_2} (q_2 - q_1) G .$$

With the physical situation in mind we introduce the following assumptions and notations:

$$(D_1 - D_2)/D_2 = \alpha \geq 0 , \quad \kappa_1^2 - \kappa_2^2 = \beta \geq 0 .$$

Other cases can be discussed in a manner similar to the analysis below. Also observe that $G > 0$, $dG(x)/dx < 0$, and

$$\gamma = \frac{1}{D_2} \left[\int_{R_{1+2}} q_1 G + \int_{R_2} (q_2 - q_1) G \right] > 0 .$$

The integral equation (I.12) now reads

$$(I.13) \quad \varphi = \alpha \int_{S_2} \varphi \frac{\partial G}{\partial n} + \beta \int_{R_2} \varphi G + \gamma \quad .$$

To apply the method of successive approximations we require a starting function φ_0 and an estimate of the error, $\epsilon_0 = \varphi_0 - \varphi$. These are most easily obtained by determining upper and lower bounds for the flux φ . The simplest bounds are the largest and smallest asymptotic values of the flux but better bounds can usually be calculated. Consider region R_2 and let φ_{\max} and φ_{\min} denote the maximum and the minimum values of φ there. The convexity assumption implies $\partial G / \partial n < 0$ on S_2 . Since α , β , and γ are non-negative, it can be concluded from (I.13) that

$$(I.14) \quad \varphi \leq \alpha \varphi_{\min} \int_{S_2} \frac{\partial G}{\partial n} + \beta \varphi_{\max} \int_{R_2} G + \gamma \quad ,$$

$$(I.15) \quad \varphi \geq \alpha \varphi_{\max} \int_{S_2} \frac{\partial G}{\partial n} + \beta \varphi_{\min} \int_{R_2} G + \gamma \quad .$$

Inequalities (I.14) and (I.15) furnish upper and lower bounds for φ at any point \underline{r} in region R_2 in terms of φ_{\max} and φ_{\min} there. In particular let \underline{r} be a point at which φ_{\max} is attained. Solving (I.14) and (I.15) for φ_{\max} gives

$$(I.16) \quad \frac{\beta \varphi_{\min} \int_{R_2} G + \gamma}{1 - \alpha \int_{S_2} \frac{\partial G}{\partial n}} \leq \varphi_{\max} \leq \frac{\alpha \varphi_{\min} \int_{S_2} \frac{\partial G}{\partial n} + \gamma}{1 - \beta \int_{R_2} G} \quad .$$

Similarly, bounds for φ_{\min} are

$$(I.17) \quad \frac{\alpha \varphi_{\max} \int_{S_2} \frac{\partial G}{\partial n} + \gamma}{1 - \beta \int_{R_2} G} \leq \varphi_{\min} \leq \frac{\beta \varphi_{\max} \int_{R_2} G + \gamma}{1 - \alpha \int_{S_2} \frac{\partial G}{\partial n}} .$$

The inequalities (I.16) and (I.17) may be manipulated in various ways. The extreme inequalities can be solved to provide a lower bound for φ_{\max} and an upper bound for φ_{\min} . Since it is apparent that $\varphi_{\min} \geq \min(q/\Sigma)$, an upper bound, Ψ , for φ_{\max} can be obtained from (I.16). Then an improved lower bound, $\bar{\Psi}$, for φ_{\min} is given by the left side of (I.17). To what extent further manipulation is desirable depends on the problem at hand.

It should be observed that the upper bound for φ_{\min} furnished by (I.16) is itself a significant number. If $q_2/\Sigma_2 > q_1/\Sigma_1$ then the facts that $D_2 \geq D_1$ and that R_2 is convex imply φ_{\min} occurs on S_2 . Also since R_2 is convex and is large enough for diffusion theory to apply, the flux would not be expected to vary greatly on the surface S_2 . These "facts" imply that the upper bound for φ_{\min} already furnishes an estimate of how much flux peaking will occur in the external region.

As a zeroth approximation to the flux we can take $\varphi_0 = (\psi + \bar{\Psi})/2$ and know the error ϵ_0 does not exceed $(\psi - \bar{\Psi})/2$. The error ϵ_1 in φ_1 can be estimated in various ways, depending on how many iterates are available. Operating on (I.10) with A gives $\epsilon_1 = A\epsilon_1 + \varphi_1 - \varphi_2$, from which it is possible to estimate ϵ_1 much as φ is estimated by (I.14) and (I.15). Alternatively, from $\varphi_1 + \epsilon_1 = \varphi_0 + \epsilon_0$ are derived the inequalities

$$\min \epsilon_0 + \varphi_0 - \varphi_1 \leq \epsilon_1 \leq \max \epsilon_0 + \varphi_0 - \varphi_1 .$$

Perhaps the simplest and most useful bounds for ϵ_1 are obtained from

$$\epsilon_1 = A\epsilon_0 = \alpha \int_{S_2} \epsilon_0 \frac{\partial G}{\partial n} + \beta \int_{R_2} \epsilon_0 G, \quad ,$$

which furnishes

$$|\epsilon_1| \leq \alpha \max |\epsilon_0| \int_{S_2} \frac{\partial G}{\partial n} + \beta \max |\epsilon_0| \int_{R_2} G, \quad ,$$

or, upon rearrangement,

$$\frac{|\epsilon_1|}{\max |\epsilon_0|} \leq (\beta - \alpha \kappa_1^2) \int_{R_2} G + \alpha \quad .$$

The error will tend to zero and the successive approximations will converge provided

$$(I.18) \quad (\beta - \alpha \kappa_1^2) \int_{R_2} G + \alpha < 1. \quad .$$

It is instructive to solve (I.18) for α .

$$\alpha < \frac{1 - \beta \int_{R_2} G}{1 - \kappa_1^2 \int_{R_2} G} = 1 + \frac{\kappa_2^2 \int_{R_2} G}{1 - \kappa_1^2 \int_{R_2} G} \quad .$$

The preceding inequality is certainly satisfied if $\alpha \leq 1$.

So far we have proved the first part of the following theorem:

Let α , β , and γ be non-negative and let the region R_2 be convex, then if $\alpha \leq 1$, the integral equation (I.12) can be solved by the method of successive approximations. But if $\alpha > 1$, the successive approximations can fail to converge for all sufficiently small regions R_2 ; or for a given region R_2 the approximations can fail to converge for all sufficiently large α .

Before proving the latter assertions we shall illustrate them in a particular case. Suppose $\beta = 0$ so that we have merely

$$\epsilon_n = \alpha \int_{S_2} \epsilon_{n-1} \frac{\partial G}{\partial n} .$$

Now let $\epsilon_{n-1} \geq \delta > 0$. Then $\epsilon_n \leq \alpha \delta \int_{S_2} \frac{\partial G}{\partial n} = \alpha \delta (-1 + \kappa_1^2 \int_{R_2} G)$. Choose

$\alpha > 1$ and R_2 so that $\epsilon_n \leq -\delta$. This will certainly be true if

$\kappa_1^2 \int_{R_2} G < (\alpha - 1)/\alpha$. But then $\epsilon_{n+1} \geq -\alpha \delta \int_{S_2} \frac{\partial G}{\partial n} \geq \delta$, and the successive

errors will never tend to zero; they will in fact increase. It seems remarkable that an arbitrarily good approximation, i.e., δ as small as you please, cannot ensure the convergence of the iterates.

A slight elaboration of the argument just given will complete the proof of the theorem. Let ϵ_{n-1} satisfy

$$0 < \delta_1 \leq \epsilon_{n-1} \leq \delta_2 .$$

Let

$$M = \max \int_{R_2} G , \quad m = \min \int_{R_2} G .$$

Then we have

$$-a \delta_2 + (a \kappa_1^2 \delta_2 + \beta \delta_1)M \leq \epsilon_n \leq -a \delta_1 + (a \kappa_1^2 \delta_1 + \beta \delta_2)M ;$$

and if M and a satisfy

$$M \leq \frac{(a-1)\delta_1}{a \kappa_1^2 \delta_1 + \beta \delta_2} ,$$

we find

$$-a \delta_2 \leq \epsilon_n \leq -\delta_1 .$$

Now we want to show that $\epsilon_{n+1} \geq \delta_1$, and that the argument can be continued. Clearly

$$a[\delta_1 - (\delta_1 \kappa_1^2 + \beta \delta_2)M] \leq \epsilon_{n+1} \leq a^2 \delta_2 .$$

Since

$$(\delta_1 \kappa_1^2 + \beta \delta_2)M \leq \frac{a-1}{a} \delta_1 ,$$

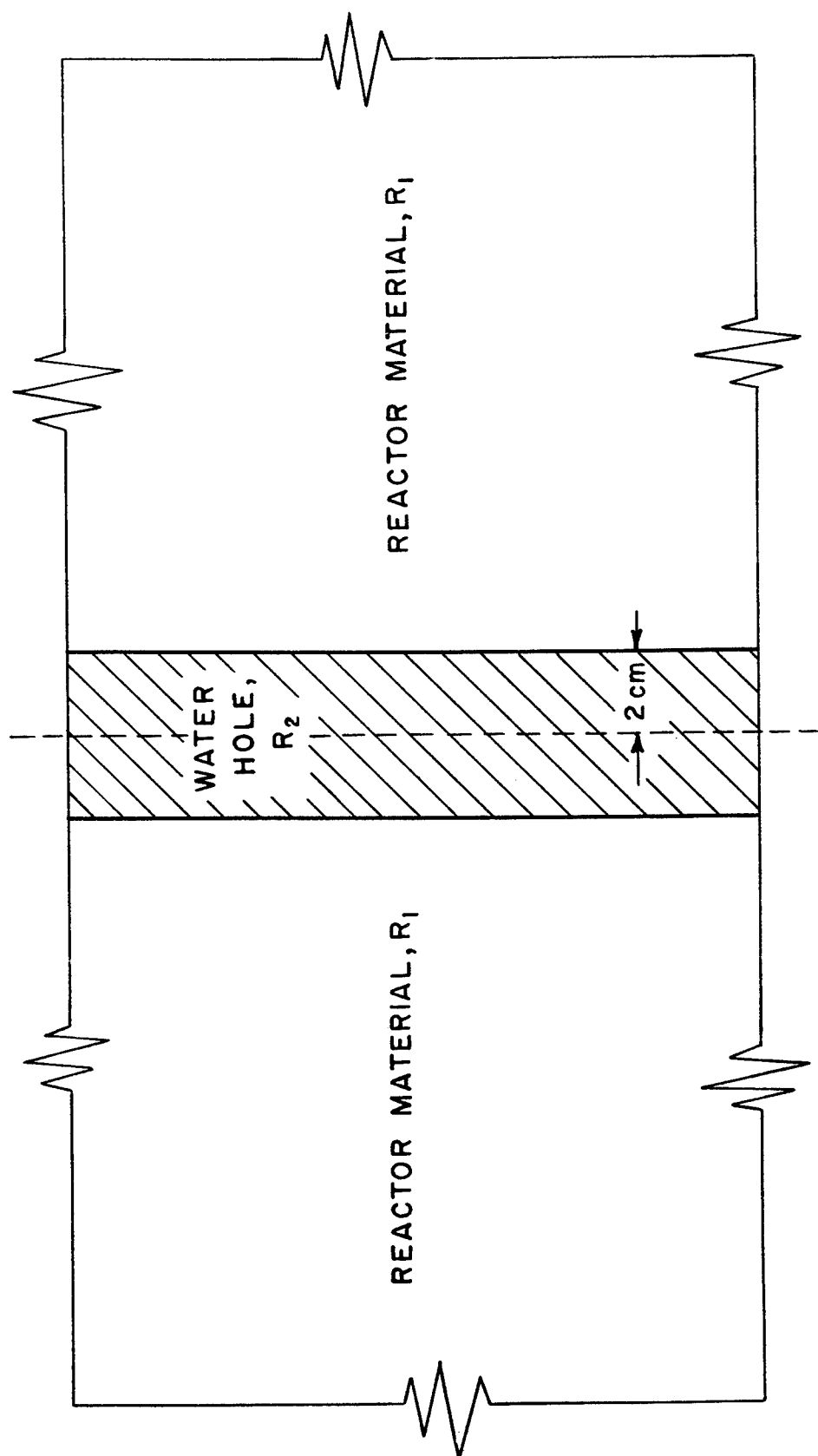
we have finally

$$\delta_1 \leq \epsilon_{n+1} \leq a^2 \delta_2 .$$

Hence

$$\begin{aligned} -a^3 \delta_2 &\leq \epsilon_{n+2} \leq -\delta_1 \\ \delta_1 &\leq \epsilon_{n+3} \leq a^4 \delta_2 \\ &\vdots \end{aligned}$$

The errors remain outside the interval $(-\delta, \delta)$, and the iterates do not converge. This completes the proof of the theorem.



SLAB WATER HOLE IN AN INFINITE REACTOR

Now that the discussion of successive approximations for a convex internal region is complete, we illustrate the application of the integral equation by determining the flux distributions in slab and cylindrical water holes.

5. The Slab Water Hole in an Infinite Reactor

In all our examples we shall use the following physical constants:

	<u>Reacting Material, R_1</u>	<u>Water Hole, R_2</u>
D	.275	.162
κ^2	.200	.121
q	1.000	2.009

Since $\alpha = (D_1 - D_2)/D_2 = .70$, the successive approximations are sure to converge.

Let the water hole, R_2 , be a slab 4 cm in thickness and let the reacting material, R_1 , extend to infinity as shown in the sketch on page 24. The flux, determined by an analytic solution of the differential equation, is

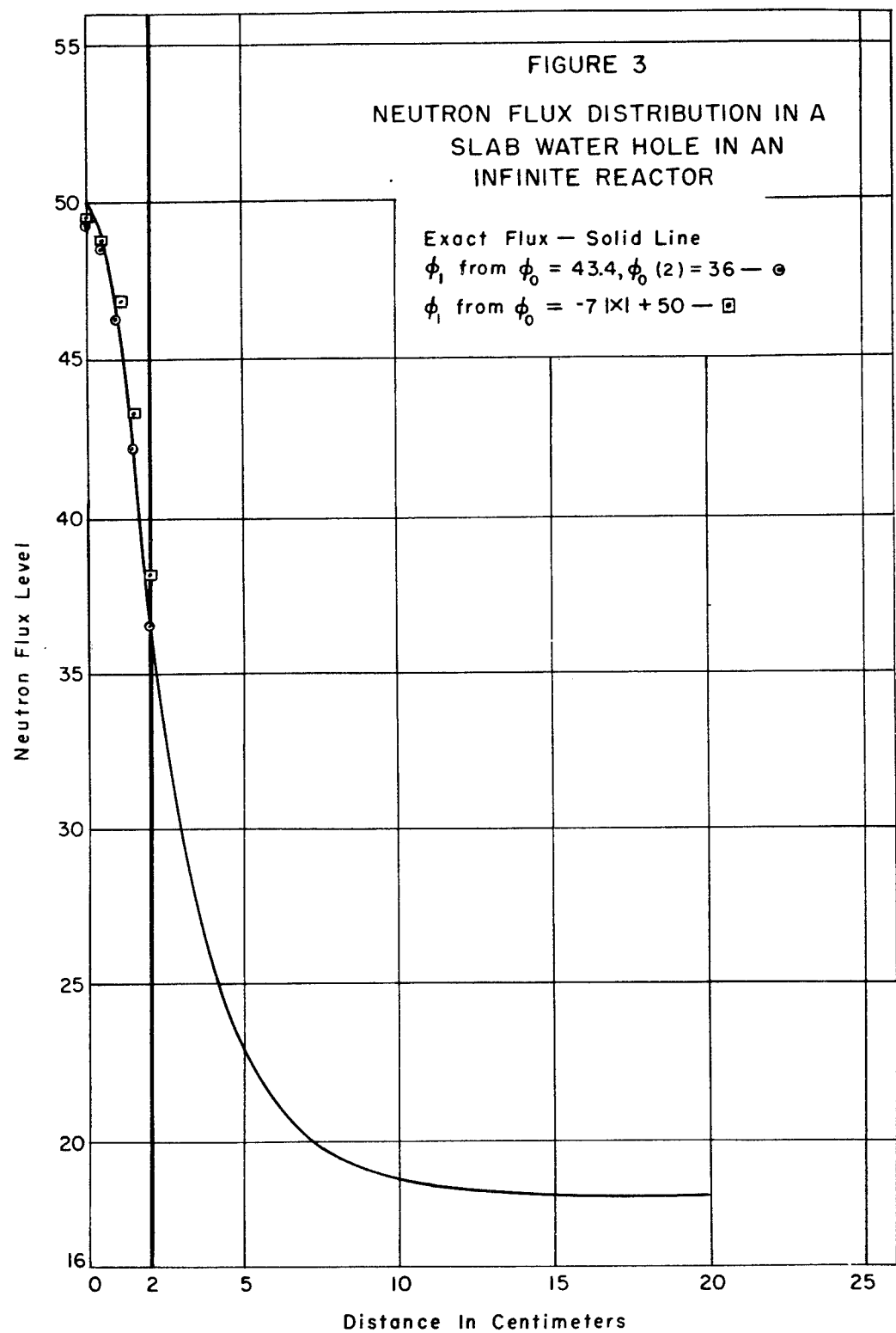
$$(1.19) \quad \varphi = \begin{cases} 44.7 e^{-.447x} + 18.2, & x \geq 2 \\ -53.1 \cosh(.347x) + 102.9, & |x| \geq 2 \end{cases}$$

This is illustrated in Figure 3, page 26.

The Green's function for the problem is

$$G(x, x') = e^{-\kappa_1 |x-x'|} / 2\kappa_1$$

and the integral equation, for φ in R_2 , reads after slight modification:



$$(I.20) \quad \varphi(x) = -\frac{D_1 - D_2}{D_2} \varphi(2) e^{-2\kappa_1} \cosh \kappa_1 x + \frac{\kappa_1^2 - \kappa_2^2}{2\kappa_1} \int_{-2}^2 \varphi(x') e^{-\kappa_1 |x-x'|} dx' \\ + \frac{q_2 - q_1}{2\kappa_1 D_2} \int_{-2}^2 e^{-\kappa_1 |x-x'|} dx' + \frac{q_1}{D_2 \kappa_1^2}.$$

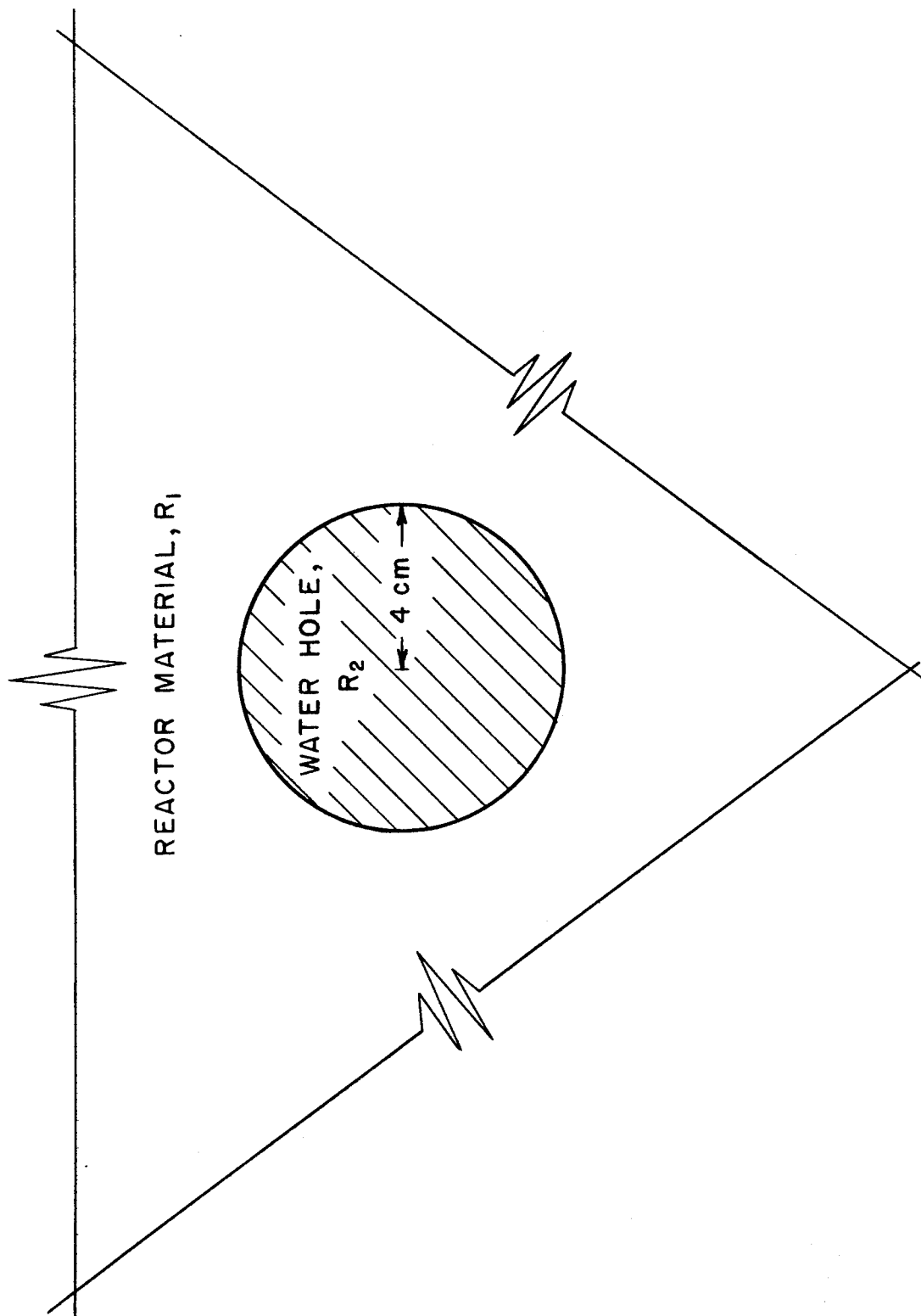
One notes that the surface integral can be explicitly evaluated in those cases in which φ is constant on the surface.

We shall calculate bounds for the flux and then obtain an approximate solution of (I.20) by iteration. As was pointed out on page 20, the maximum and minimum values of the flux in the water hole occur at $x = 0$ and $x = 2$. The right side of (I.20) is made smaller if $\varphi(x)$ is replaced by $\varphi(2)$. Then putting $x = 2$, (I.20) can be rearranged to provide the lower bound $\varphi(2) \geq 35.4$. Next put $x = 0$ and replace $\varphi(2)$ by the lower bound 35.4. This gives $\varphi(0) \leq 51.3$. An upper bound, 37.2, for $\varphi(2)$ is obtained by putting $x = 2$ and replacing $\varphi(x')$ by its majorant, 51.3. Finally $\varphi(0) \geq 47.6$ follows on replacing $\varphi(2)$ by 37.2 and $\varphi(x')$ by 35.4. In summary

$$\begin{array}{ll} 47.6 \leq \varphi(0) \leq 51.3 & \left\{ \begin{array}{l} \varphi(0) = 49.8 \\ \varphi(2) = 36.5 \end{array} \right\} \\ 35.4 \leq \varphi(2) \leq 37.2 & \end{array}.$$

It is in a way surprising that such narrow bounds for the flux at the center and at the boundary are obtained. This fact results, perhaps, from the geometry which tells us that the flux has a constant minimum value at the surface of the water hole. For many purposes, the fact that φ on the surface lies between 35 and 37 is all the information required. Since the asymptotic value of the flux is 18.2, the peaking effect of the water hole is well-defined.

A first approximation, φ_1 , to the flux has been calculated in two ways. First, put $\varphi_0(x) = 43.4$, $-2 \leq x \leq 2$, and $\varphi_0(2) = 36$. The values of $\varphi_1(x)$ calculated from (I.20) are shown as circles in Figure 3 (page 26). The approximation $\varphi_0 = 43.4$ is very rough, yet $\varphi_1(x)$ turns out to be close to the actual flux.



CYLINDRICAL WATER HOLE IN AN INFINITE REACTOR

This is due in part to the fact that a good approximation for the flux at the surface is available.

A much better initial approximation, ϕ_0 , should be given by a line segment passing through the flux values 50 and 36 at $x = 0$ and $x = 2$ respectively. For $\phi_0(x)$ we have $\phi_0 = -7|x| + 50$, with $|x| \leq 2$. The values of $\phi_1(x)$ obtained in this way are shown as squares in Figure 3 (page 26). Evidently the more elaborate estimate of ϕ_1 was not worth the effort.

6. The Cylindrical Water Hole in an Infinite Reactor

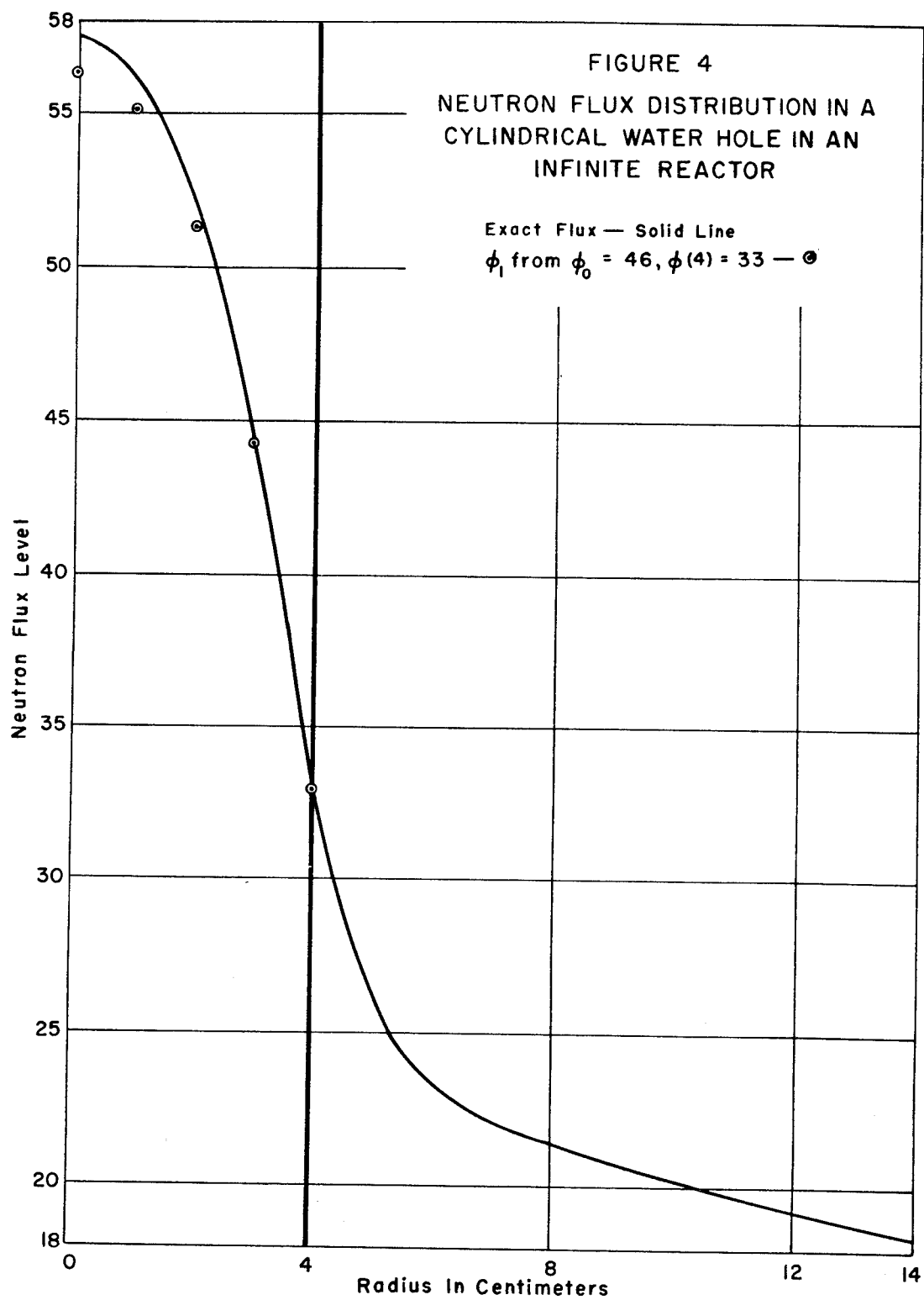
The flux distribution in a cylindrical water hole (see sketch on page 28), 8 cm in diameter, was examined by means of the integral equation. The Green's function is $K_0(\kappa_1|\underline{r} - \underline{r}'|)/2\pi$; the constants are the same as in the slab treated above. For the integral equation we now have

$$(I.21) \quad \phi(r) = \frac{D_1 - D_2}{D_2} \frac{\phi(4)}{2\pi} \int_{S_2} \frac{\partial K_0}{\partial n} + \frac{(\kappa_1^2 - \kappa_2^2)}{2\pi} \int_{R_2} \phi(\underline{r}') K_0(\kappa_1|\underline{r} - \underline{r}'|) \\ + \frac{q_1 - q_2}{2\pi D_2} \int_{R_2} K_0(\kappa_1|\underline{r} - \underline{r}'|) + \frac{q_1}{D_2 \kappa_1^2} \quad .$$

The surface integral in (I.21) is transformed to a volume integral by Green's theorem. Expansion of $K_0(\kappa_1|\underline{r} - \underline{r}'|)$ by the addition theorem for Bessel's functions and integration over the angular variable replaces the double integrals by simple integrals which are manageable.

The exact analytical solution of (I.21) is

$$(I.22) \quad \phi(r) = \begin{cases} -45.5 I_0(.347r) + 102.9 & , & r \leq 4 \\ 98.3 K_0(.447r) + 18.2 & , & r \geq 4 \end{cases} .$$



Bounds for $\varphi_{\min} = \varphi(4)$ and $\varphi_{\max} = \varphi(0)$ are found exactly as before.

$$\begin{array}{ll} 31.6 \leq \varphi(4) \leq 34.3 & , \\ 52.2 \leq \varphi(0) \leq 60.5 & , \end{array} \quad \left\{ \begin{array}{l} \varphi(4) = 32.8 \\ \varphi(0) = 57.5 \end{array} \right\} .$$

The first approximation $\varphi_1(r)$ was calculated from $\varphi_0 = 46$, $\varphi(4) = 33$. The iterated flux φ_1 , as well as the correct flux φ , is illustrated in Figure 4 (page 30).

7. Non-Convex Regions

The question of convergence of the successive approximations is by no means simple for regions that are not convex. For purposes of computation it is not only the fact of convergence which is important; equally important is the requirement that the successive approximations converge rapidly. It is easy to see that no general criteria can ensure the convergence in a manner which is useful. In equation (I.13), let $\beta = 0$. We prove:

For every $\alpha > 0$ there exist regions, R_2 , such that the iterated error ϵ_1 is at some point arbitrarily large, although ϵ_0 is as small as you please.

There is no loss in generality in allowing ϵ_0 to be discontinuous. With respect to some point in a region, R_2 , let $\epsilon_0 = \delta > 0$ on that part of the surface where $\partial G / \partial n > 0$ and let $\epsilon_0 = -\delta$ where $\partial G / \partial n < 0$. Then

$$\epsilon_1 = \alpha \delta \int_{S_2} \left| \frac{\partial G}{\partial n} \right| .$$

Clearly there exist non-convex regions such that $\int_{S_2} \left| \frac{\partial G}{\partial n} \right|$ is, for some point,

greater than any preassigned number. This proves the assertion. Of course, the counter example is pathological; one can hope that ordinarily the process of iteration will not lead to disastrous results.

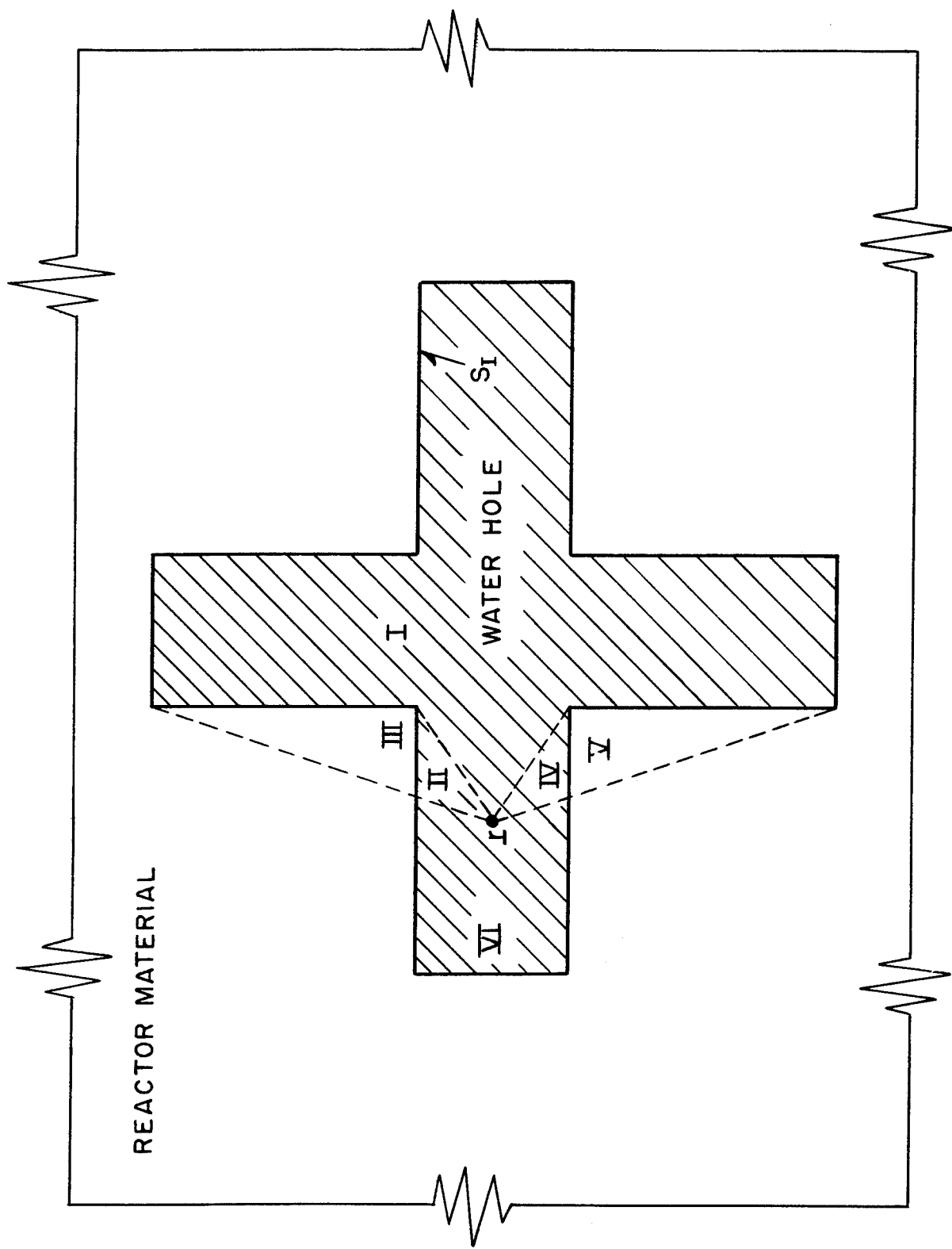


FIGURE 5
CROSS-SHAPED WATER HOLE IN AN INFINITE REACTOR

What we can say is that $|\epsilon_n|$ will certainly tend steadily to zero if

$$(I.23) \quad \frac{|\epsilon_n|}{\max |\epsilon_{n-1}|} \leq \alpha \int_{S_2} \left| \frac{\partial G}{\partial n} \right| + \beta \int_{R_2} G < 1.$$

The only way of improving on (I.23) is to obtain some knowledge of the distribution of the error on the surface. One way of doing this is to obtain bounds for ϕ at various points on the surface from the inequalities analogous to (I.14) and (I.15) which are applicable to non-convex bodies. These inequalities will be derived, for the cross-shaped water hole, in the next section.

8. The Cross-Shaped Water Hole in an Infinite Reactor

Our interest here is to show one way in which bounds for the flux in non-convex regions can be calculated. The cross-shaped water hole is used only for purposes of illustration. We already know an upper and a lower bound for the flux--the asymptotic flux values. Other bounds can be obtained by modifying the physical constants to yield simpler integral equations whose solutions are everywhere greater than or less than the correct flux. Our procedure here will be to obtain inequalities analogous to those derived in section 4 for convex regions. Let the point of interest be \underline{r} , Figure 5 (page 32), and draw the auxiliary surfaces shown by the dotted lines. In addition to the cross R_2 and surface S_2 , we consider the six regions R_I, \dots, R_{VI} and surfaces S_I, \dots, S_{VI} . All normals are directed outward. From the equality,

$$\int_{S_2} = \int_{S_2+S_{III}+S_V} + \int_{S_{II}+S_{IV}} - \int_{S_{II}+S_{III}+S_{IV}+S_V}$$

follow

$$(I.24) \quad \int_{S_2} \varphi \frac{\partial G}{\partial n} \leq \varphi_{\min} \int_{S_2+S_{III}+S_V} \frac{\partial G}{\partial n} + \varphi_{\min} \int_{S_{II}+S_{IV}} \frac{\partial G}{\partial n} - \varphi_{\max} \int_{S_{II}+S_{III}+S_{IV}+S_V} \frac{\partial G}{\partial n} ,$$

and

$$(I.25) \quad \int_{S_2} \varphi \frac{\partial G}{\partial n} \geq \varphi_{\max} \int_{S_2+S_{III}+S_V} \frac{\partial G}{\partial n} + \varphi_{\max} \int_{S_{II}+S_{IV}} \frac{\partial G}{\partial n} - \varphi_{\min} \int_{S_{II}+S_{III}+S_{IV}+S_V} \frac{\partial G}{\partial n} ,$$

where, in the first instance, the maximum and minimum values of φ are to be taken on the appropriate surfaces.

These inequalities appear to better advantage when rearranged thus:

$$(I.26) \quad \int_{S_2} \varphi \frac{\partial G}{\partial n} \leq \varphi_{\min} \int_{S_2} \frac{\partial G}{\partial n} + (\varphi_{\min} - \varphi_{\max}) \int_{S_{II}+S_{III}+S_{IV}+S_V} \frac{\partial G}{\partial n} ,$$

$$(I.27) \quad \int_{S_2} \varphi \frac{\partial G}{\partial n} \geq \varphi_{\max} \int_{S_2} \frac{\partial G}{\partial n} + (\varphi_{\max} - \varphi_{\min}) \int_{S_{II}+S_{III}+S_{IV}+S_V} \frac{\partial G}{\partial n}$$

From (I.26), (I.27), and the integral equation (I.13) are obtained the bounds, for φ in the cross,

$$(I.28) \quad \varphi \leq \alpha \varphi_{\min} \int_{S_2} \frac{\partial G}{\partial n} + \alpha(\varphi_{\min} - \varphi_{\max}) \int_{S_{II}+S_{III}+S_{IV}+S_V} \frac{\partial G}{\partial n} + \beta \varphi_{\max} \int_{R_2} G + \gamma ,$$

$$(I.29) \quad \varphi \geq \alpha \varphi_{\max} \int_{S_2} \frac{\partial G}{\partial n} + \alpha(\varphi_{\max} - \varphi_{\min}) \int_{S_{II}+S_{III}+S_{IV}+S_V} \frac{\partial G}{\partial n} + \beta \varphi_{\min} \int_{R_2} G + \gamma .$$

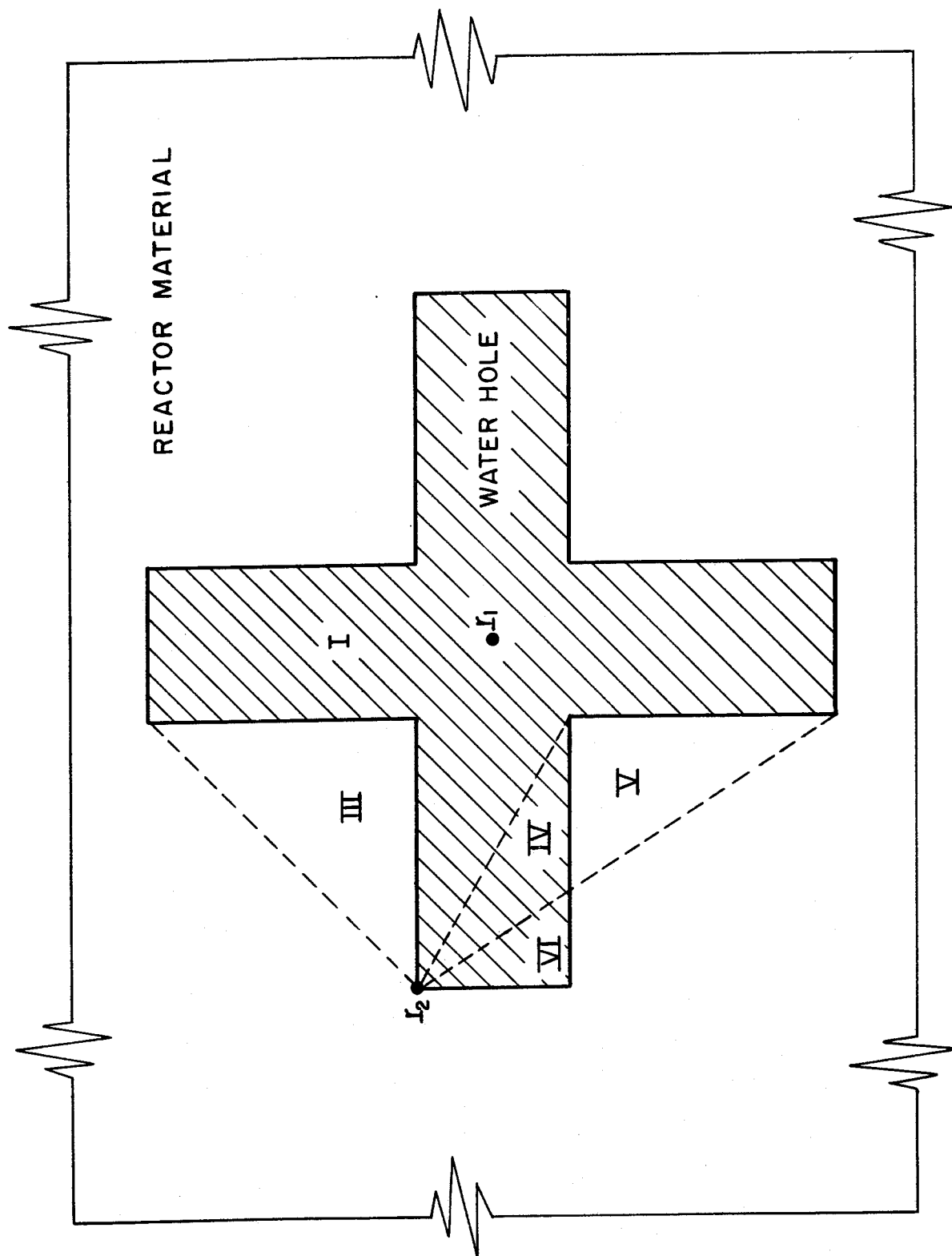


FIGURE 6
CROSS-SHAPED WATER HOLE IN AN INFINITE REACTOR

The right hand sides of (I.28) and (I.29) are unambiguous if φ_{\max} and φ_{\min} are understood to be the maximum and minimum values of φ in the entire region $R_I + \dots + R_{VI}$; the inequalities are sharper if φ_{\min} and φ_{\max} are interpreted to best advantage each place they occur.

Now we shall suppose that φ_{\max} occurs at the center of the cross, \underline{r}_1 , and that φ_{\min} (in the cross) occurs at the corner \underline{r}_2 , Figure 6 (page 35). At the point \underline{r}_1 , $\partial G / \partial n$ is everywhere negative, i.e., the cross looks convex from the center. Therefore inequalities (I.16) apply with $\varphi_{\max} = \varphi(\underline{r}_1)$ and $\varphi_{\min} = \varphi(\underline{r}_2)$.

The only lower bound available for φ in regions R_{III} and R_V is the asymptotic value q_1 / \sum_1 . The sharpest bounds for $\varphi(\underline{r}_2)$ are obtained by using (I.24) and (I.25):

$$(I.30) \quad \varphi(\underline{r}_2) \leq \alpha \frac{q_1}{\sum_1} \int_{S_2+S_{III}+S_V} \frac{\partial G}{\partial n} + \alpha \varphi(\underline{r}_2) \int_{S_{IV}} \frac{\partial G}{\partial n} - \alpha \varphi(\underline{r}_0) \int_{S_{III}+S_{IV}+S_V} \frac{\partial G}{\partial n} \\ + \beta \varphi(\underline{r}_0) \int_{R_2} G + \gamma \quad ,$$

$$(I.31) \quad \varphi(\underline{r}_2) \geq \alpha \varphi(\underline{r}_0) \int_{S_2+S_{III}+S_{IV}+S_V} \frac{\partial G}{\partial n} - \alpha \frac{q_1}{\sum_1} \int_{S_{III}+S_{IV}+S_V} \frac{\partial G}{\partial n} + \beta \varphi(\underline{r}_2) \int_{R_2} G + \gamma \quad .$$

Solving (I.30) and (I.31) for $\varphi(\underline{r}_2)$ then gives the inequalities we set out to derive:

$$\begin{aligned}
(I.32) \quad & \frac{\alpha \varphi(r_0) \int_{S_2+S_{III}+S_{IV}+S_V} \frac{\partial G}{\partial n} - \alpha \frac{q_1}{\sum_1} \int_{S_{III}+S_{IV}+S_V} \frac{\partial G}{\partial n} + \gamma}{1 - \beta \int_{R_2} G} \leq \varphi(r_2) \leq \\
& \frac{\alpha \frac{q_1}{\sum_1} \int_{S_2+S_{III}+S_{IV}+S_V} \frac{\partial G}{\partial n} - \alpha \varphi(r_0) \int_{S_{III}+S_{IV}+S_V} \frac{\partial G}{\partial n} + \beta \varphi(r_0) \int_{R_2} G + \gamma}{1 - \alpha \int_{S_{IV}} \frac{\partial G}{\partial n}}.
\end{aligned}$$

With these cumbersome inequalities we end our discussion of non-convex regions. In a later report we hope to give comprehensive numerical results illustrating the methods discussed in this report in their application to cross-shaped water holes.

Before turning to the very important method of superposition, we make an observation on the boundary values satisfied by the flux in the internal region R_2 .

9. Appendix to Part I

As was pointed out before, the integral equation (I.12) for the flux in R_2 can be solved without any consideration of the flux in R_1 . Since φ satisfies the differential equation (I.3) it is natural to ask whether or not the integral equation (I.12) is equivalent to the differential equation and a boundary condition on S_2 which involves only the flux in R_2 . This question will be examined here.

From the equations

$$(I.3) \quad D_2 \nabla^2 \varphi - \sum_2 \varphi + q_2 = 0$$

$$(I.5) \quad D_1 \nabla^2 G - \sum_1 G = 0 ,$$

is obtained at once the integral equation

$$(I.33) \quad D_2 \varphi = D_2 \int_{S_2} (G \frac{\partial \varphi}{\partial n} - \varphi \frac{\partial G}{\partial n}) + (\kappa_1^2 - \kappa_2^2) D_2 \int_{R_2} G \varphi + q_2 \int_{R_2} G .$$

Certainly this integral equation cannot determine φ since no boundary condition has been imposed. Now equation (I.33) could be transformed to yield (I.12) if the boundary condition were known. Hence the boundary condition must be implicit in the equation obtained by subtracting (I.33) from (I.12). There results

$$D_1 \int_{S_2} \varphi \frac{\partial G}{\partial n} - D_2 \int_{S_2} G \frac{\partial \varphi}{\partial n} + q_1 \int_{R_1} G = 0$$

or

$$(I.34) \quad \int_{S_2} \left[D_1 \left(\varphi - \frac{q_1}{\sum_1} \right) \frac{\partial G}{\partial n} - D_2 G \frac{\partial \varphi}{\partial n} \right] = 1 - \kappa_1^2 \int_{R_{1+2}} G$$

The preceding line is indeed a boundary condition, a very complicated boundary condition. It asserts that we must select from all the solutions of (I.3) the one whose boundary values make (I.34) an identity as a function of \underline{r} .

Suppose S_2 and S are concentric cylinders with radii a and b respectively. Then φ and $\partial\varphi/\partial n$ are constant on S_2 and the boundary condition reads

$$\left[D_1 \varphi(a) - \frac{q_1}{\Sigma_1} \right] \int_{S_2} \frac{\partial G}{\partial n} - D_2 \varphi'(a) \int_{S_2} G = 1 - \kappa_1^2 \int_{R_{1+2}} G .$$

Now put $r = 0$. Then

$$G(r') = \frac{1}{2\pi} \left[K_0(\kappa_1 r') - \frac{K_0(\kappa_1 b)}{I_0(\kappa_1 b)} I_0(\kappa_1 r') \right] ,$$

$$\int_{R_{1+2}} G = \frac{1}{\kappa_1^2} \left[1 - \frac{1}{I_0(\kappa_1 b)} \right] ,$$

$$\int_{S_2} \frac{\partial G}{\partial n} = -\kappa_1 \left[K_1(\kappa_1 a) - \frac{K_0(\kappa_1 b)}{I_0(\kappa_1 b)} I_1(\kappa_1 a) \right] ,$$

so that the boundary condition becomes

$$(I.35) \quad D_1 \kappa_1 \left[\frac{K_1(\kappa_1 a)}{K_0(\kappa_1 b)} + \frac{I_1(\kappa_1 a)}{I_0(\kappa_1 b)} \right] \left[\varphi(a) - \frac{q_1}{\Sigma_1} \right] \\ + D_2 \left[\frac{K_0(\kappa_1 a)}{K_0(\kappa_1 b)} - \frac{I_0(\kappa_1 a)}{I_0(\kappa_1 b)} \right] \varphi'(a) = -\frac{1}{I_0(\kappa_1 b)} .$$

In particular, if $b = \infty$,

$$D_1 \kappa_1 K_1(\kappa_1 a) + D_2 K_0(\kappa_1 a) \varphi'(a) - \frac{q_1}{\kappa_1} K_1(\kappa_1 a) = 0$$

Of course, the boundary condition (I.35) may be derived in a completely elementary manner.

II. THE METHOD OF SUPERPOSITION

Numerical solution of the integral equation for complicated configurations is a formidable task. The difficulties are of two kinds. The first of these is typified by the problem of many water holes in an infinite reactor, or even of a single water hole with a complicated shape. Difficulties of another kind enter into the calculations when the reactor does not extend to infinity. For then we are faced with an unwieldy Green's function, if it is known at all, and with source terms which cannot be considered constant in each homogeneous part of the system. These obstacles are largely overcome by the use of the method of superposition, a procedure which has often been applied, implicitly if not explicitly.

Consider two water holes in an infinite reactor. Let $\varphi^{(2)}$ and $\varphi^{(3)}$ be the flux distributions due to each in the absence of the other one. Let q_1/Σ_1 be the asymptotic value of the flux. By superposition we mean the flux distribution

$$\varphi^{(s)} = \varphi^{(2)} + \varphi^{(3)} - (q_1/\Sigma_1) \quad .$$

The question to be answered is how well does $\varphi^{(s)}$ approximate the correct flux distribution φ .

The term superposition will be used also in another sense. Let ψ be the flux distribution for a water hole in a reactor which extends to infinity. Can the flux distribution for the same water hole in a finite reactor be reasonably well described by the product

$$\varphi^{(s)} = \psi F$$

where F is a suitable weighting function, usually easily determined? We shall refer to the two kinds of superposition as superposition by addition and superposition by multiplication.

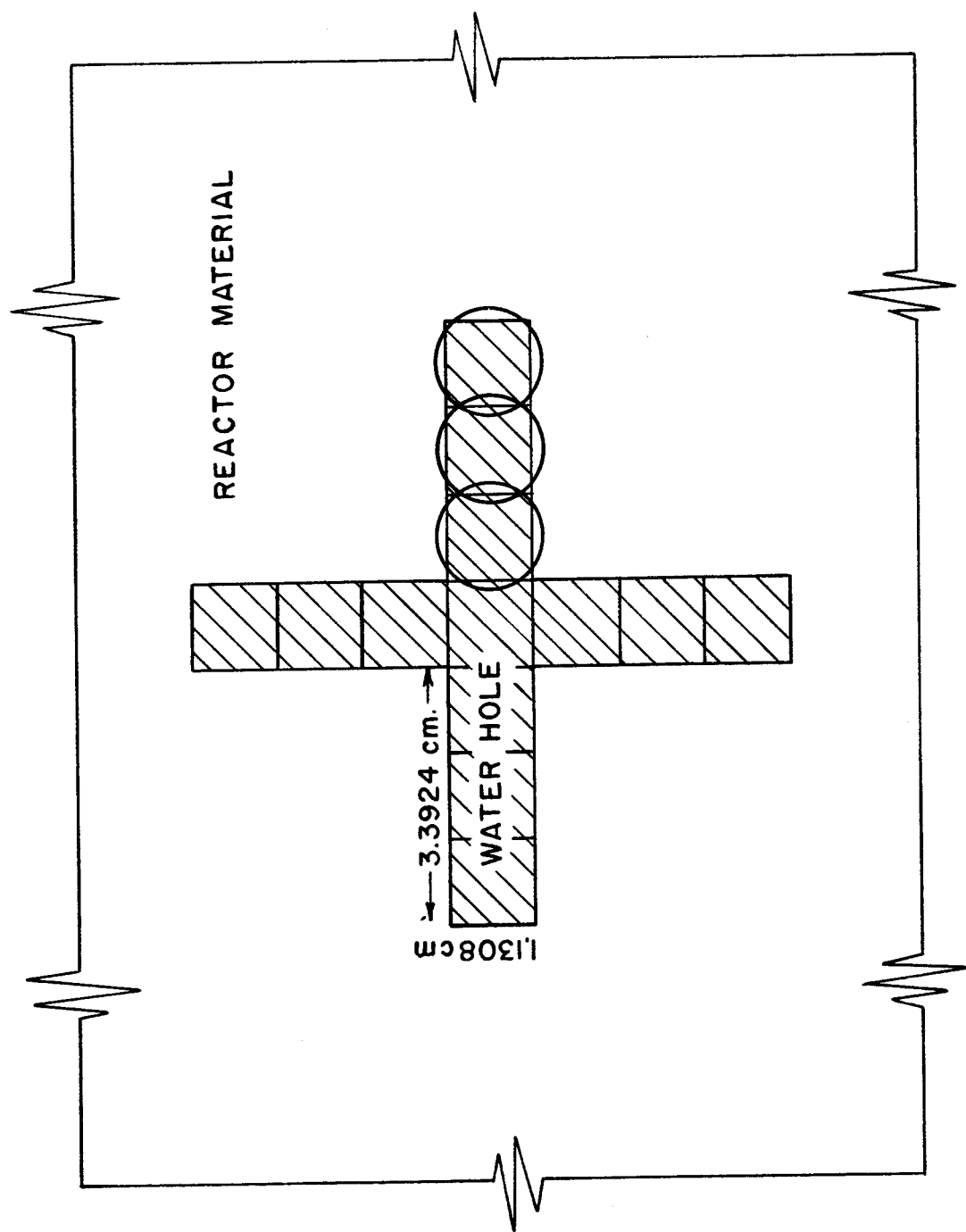


FIGURE 7

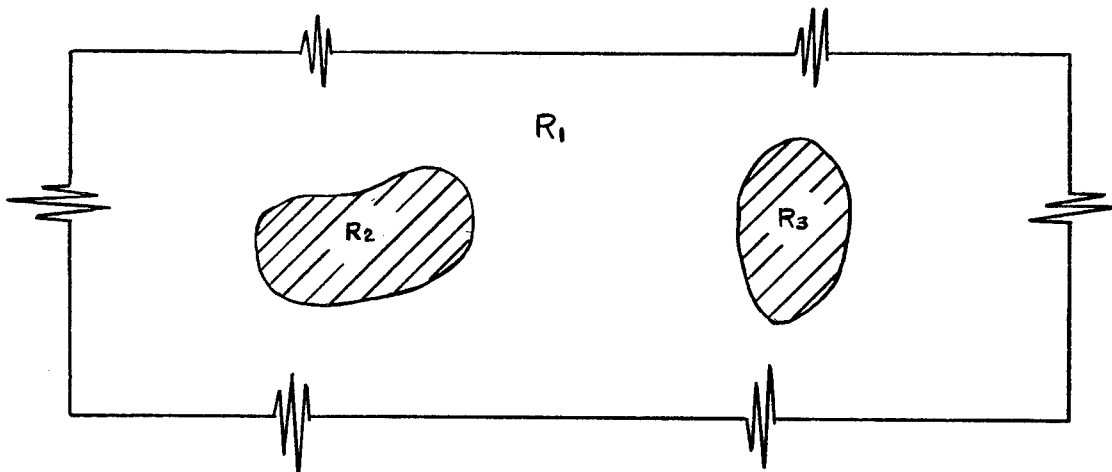
APPROXIMATION TO THE CROSS-SHAPED WATER
HOLE BY CYLINDERS

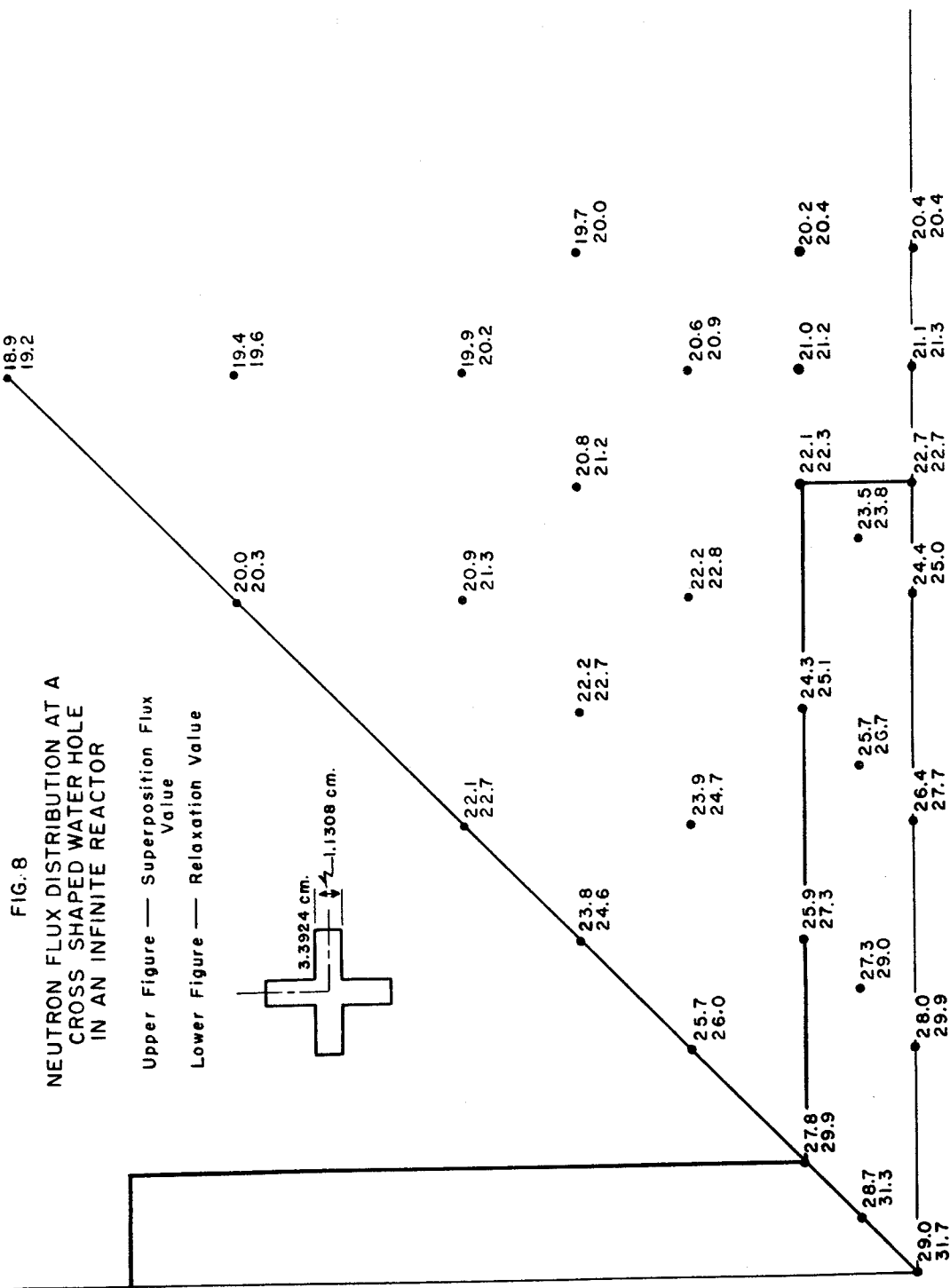
More convincing than any abstract mathematical discussion of the power of superposition is the drastic test provided by breaking up the cross shaped water hole into cylinders and superimposing the flux distribution of the cylinders. The cross section of the cross shaped water hole we are considering can be thought of as made up of 13 squares, Figure 7. The method of superposition used was to replace each square by a circle of equal area and to superimpose the flux distributions of the circles. The correct flux values as well as the values obtained by superposition are plotted in Figure 8 (page 43). In this case superposition underestimates the flux. The error in $\phi - (q_1/\Sigma_1)$, the flux rise over the asymptotic value, is less than 20%. As will be shown below, the fact of underestimation can be predicted and a correction can be applied.

Formulae which justify the method of superposition and which can be used to estimate the superposition error will now be derived. Also a simple first order correction to superposition is obtained. In section 1, superposition by addition is discussed and illustrated by finite slab water holes in an infinite reactor. Multiplicative superposition is discussed in section 2, where we take as our example a slab water hole in a finite slab reactor. In section 3 a finite reactor with internal and external reflectors is considered briefly.

1. Superposition by Addition

We shall examine the flux distributions created by two diffusing regions R_2 and R_3 in an infinite medium R_1 , as illustrated.





The flux φ is the solution of the integral equation

$$(II.1) \quad D_i \varphi = L(\varphi) + Q$$

where

$$(II.2) \quad L(\varphi) = (D_1 - D_2) \int_{S_2} \varphi \frac{\partial G}{\partial n} + (D_1 - D_3) \int_{S_3} \varphi \frac{\partial G}{\partial n} \\ + (\kappa_1^2 - \kappa_2^2) D_2 \int_{R_2} G \varphi + (\kappa_1^2 - \kappa_3^2) D_3 \int_{R_3} G \varphi ,$$

and

$$Q = \int_{R_{1+2+3}} q_1 G + \int_{R_2} (q_2 - q_1) G + \int_{R_3} (q_3 - q_1) G .$$

Let $\varphi^{(2)}$ and $\varphi^{(3)}$ be the flux distributions due to media R_2 and R_3 separately. Then

$$D_i \varphi^{(j)} = (D_1 - D_j) \int_{S_j} \varphi^{(j)} \frac{\partial G}{\partial n} + (\kappa_1^2 - \kappa_j^2) D_j \int_{R_j} G \varphi^{(j)} \\ + \int_{R_{1+2+3}} q_1 G + \int_{R_j} (q_j - q_1) G , \quad \begin{matrix} j = 2, 3 \\ i = 1, \text{ or } j . \end{matrix}$$

Let $\varphi^{(s)} = \varphi^{(2)} + \varphi^{(3)} - q_1 / \Sigma_1$ be the superposed flux. We want to estimate $\delta \varphi = \varphi - \varphi^{(s)}$. It can be verified that $\delta \varphi$ satisfies the following integral equation

$$(II.3) \quad D_i \delta \varphi = L(\delta \varphi) + \delta Q , \quad i = 1, 2, 3 ,$$

where the operator L is defined in (II.2) and

$$\begin{aligned}
 \text{(II.4)} \quad \delta Q = & (D_1 - D_2) \int_{S_2} \left[\varphi^{(3)} - \frac{q_1}{\Sigma_1} \right] \frac{\partial G}{\partial n} + (D_1 - D_3) \int_{S_3} \left[\varphi^{(2)} - \frac{q_1}{\Sigma_1} \right] \frac{\partial G}{\partial n} \\
 & + (\kappa_1^2 - \kappa_2^2) D_2 \int_{R_2} \left[\varphi^{(3)} - \frac{q_1}{\Sigma_1} \right] G + (\kappa_1^2 - \kappa_3^2) D_3 \int_{R_3} \left[\varphi^{(2)} - \frac{q_1}{\Sigma_1} \right] G \\
 & + (D_1 - D_i) \left[\varphi^{(i+(-1)^i)} - (q_1/\Sigma_1) \right] .
 \end{aligned}$$

Equation (II.3) is an inhomogeneous integral equation which differs from (II.1) only in the inhomogeneous term δQ . If δQ were zero then $\delta\varphi = 0$ and superposition would give the correct answer. Note that (II.4) states that the extent to which δQ differs from zero depends on the deviations of the fluxes $\varphi^{(2)}$ and $\varphi^{(3)}$ from their asymptotic values in regions R_3 and R_2 respectively.

The superposition flux $\varphi^{(s)}$ is that approximation to φ in which $\delta\varphi = 0$. Now $\delta\varphi = 0$ can be thought of as a zeroth approximation in solving (II.3) by iteration; hence a first approximation, $\delta\varphi_1$, to $\delta\varphi$ is obtained by putting $\delta\varphi = 0$ in the right hand side of (II.3). There results

$$\delta\varphi_1 = \delta Q / D_i ,$$

but it does not necessarily follow that $\varphi^{(s)} + \delta\varphi_1$ is a better approximation to φ than $\varphi^{(s)}$. It can only be hoped that the iterate is more nearly correct than the zeroth approximation. The correction is in the right direction, for it can be assumed that $\delta\varphi$ will have the sign of δQ , at least if δQ is either everywhere positive or everywhere negative.

The sign of δQ in the internal regions can be determined for certain problems of importance. Let the point of interest, \underline{r} , be in R_2 . Now we make

the assumption R_2 is convex so that $\partial G/\partial n$ is negative on S_2 . Put $\varphi^{(i)} - (q_1/\Sigma_1) = \Delta\varphi^{(i)}$. Then, if $\alpha = (D_1 - D_2)/D_2 \geq 0$, $\beta = \kappa_1^2 - \kappa_2^2 \geq 0$, we have

$$\begin{aligned} \frac{\delta Q}{D_2} &\leq \alpha \int \max_{R_2} \Delta\varphi^{(3)} - \min_{S_2} \Delta\varphi^{(3)} \int \\ &\quad + \int \beta \max_{R_2} \Delta\varphi^{(3)} + \kappa_1^2 \alpha \min_{S_2} \Delta\varphi^{(3)} \int_{R_2} G + \frac{\epsilon}{D_2} \quad , \end{aligned}$$

$$\begin{aligned} \frac{\delta Q}{D_2} &\geq \alpha \int \min_{R_2} \Delta\varphi^{(3)} - \max_{S_2} \Delta\varphi^{(3)} \int \\ &\quad + \int \beta \min_{R_2} \Delta\varphi^{(3)} + \kappa_1^2 \alpha \max_{S_2} \Delta\varphi^{(3)} \int_{R_2} G + \frac{\epsilon}{D_2} \quad , \end{aligned}$$

where ϵ is the contribution of the terms containing the integrals over S_3 and R_3 . In deriving these inequalities it must be remembered that our assumptions imply $\Delta\varphi^{(3)} > 0$.

For $\alpha > 0$ it follows that $\delta Q \leq 0$ in R_2 if

$$(II.5) \quad \frac{\max_{R_2} \Delta\varphi^{(3)}}{\min_{S_2} \Delta\varphi^{(3)}} \leq \frac{1 - \kappa_1^2 \int_{R_2} G}{1 + \frac{\beta}{\alpha} \int_{R_2} G} - \frac{\epsilon/D_2}{\min_{S_2} \Delta\varphi^{(3)} (\alpha + \beta \int_{R_2} G)} ;$$

and $\delta Q \geq 0$ in R_2 if

$$(II.6) \quad \frac{\min_{R_2} \Delta\varphi^{(3)}}{\max_{S_2} \Delta\varphi^{(3)}} \geq \frac{1 - \kappa_1^2 \int_{R_2} G}{1 + \frac{\beta}{\alpha} \int_{R_2} G} - \frac{\epsilon/D_2}{\max_{S_2} \Delta\varphi^{(3)} (\alpha + \beta \int_{R_2} G)} .$$

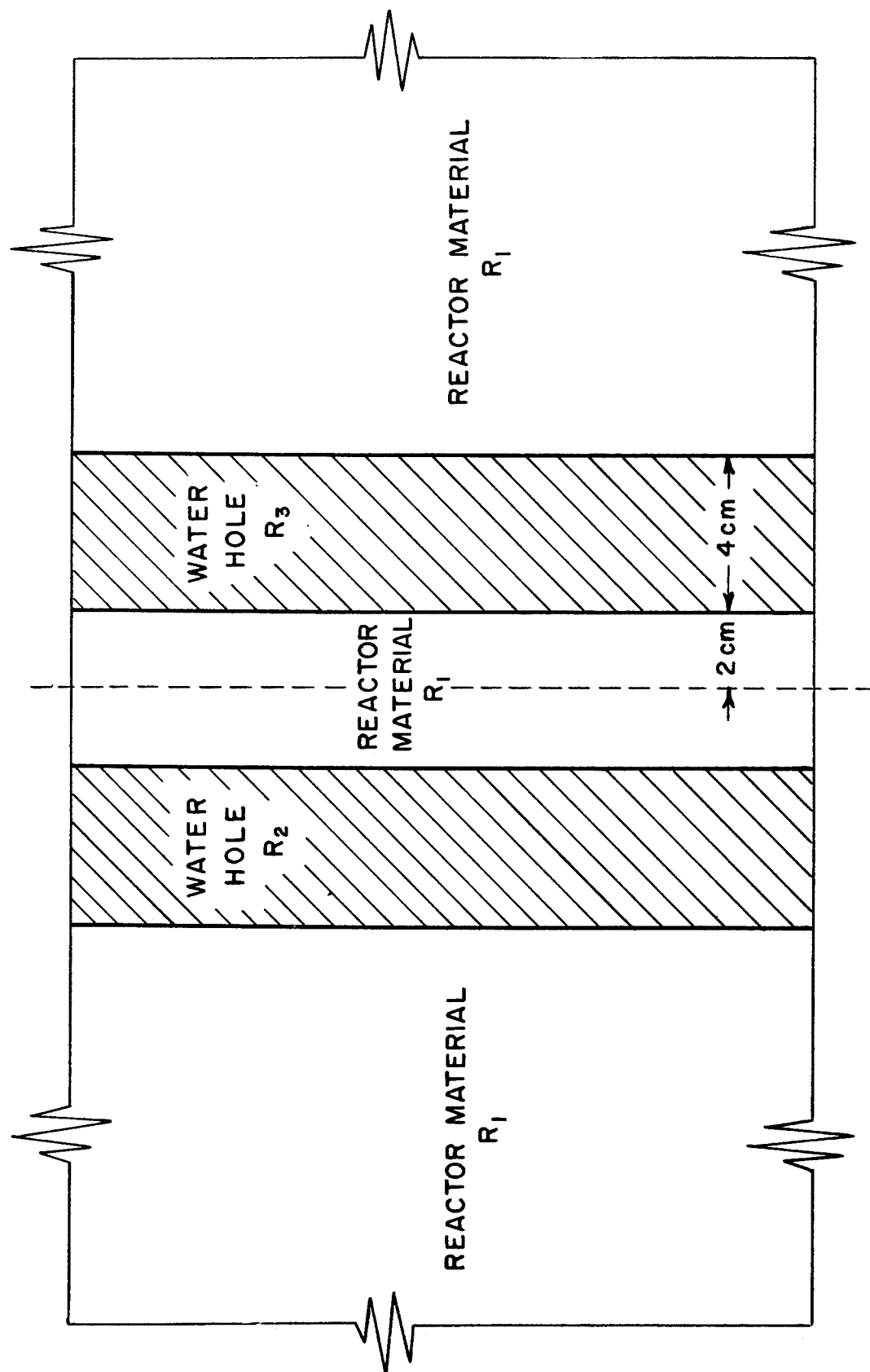
The criteria (II.5) and (II.6) are exact, but their usefulness depends upon an estimation of ϵ . In many cases the integrals over S_3 and R_3 will be negligible compared with those over S_2 and R_2 so that the terms containing ϵ can be ignored. The important contributions to the integrals over S_3 and R_3 will come from that region of R_3 nearest to R_2 since G , $\partial G/\partial n$, and $\Delta\phi^{(2)}$ all decrease rapidly with distance. Thus an approximation to ϵ is obtained if one replaces, in both integrals, $\Delta\phi^{(2)}$ by a suitable average $\overline{\Delta\phi}^{(2)}$ which is approximately the value at the nearest point. Then we find

$$\epsilon \approx (\Sigma_1 - \Sigma_3) \overline{\Delta\phi}^{(2)} \int_{R_3} G, \quad ,$$

and ϵ has the sign of $\Sigma_1 - \Sigma_3$.

The inequality (II.5) can be satisfied only if ϵ is negative and, in absolute value, not too small. On the other hand, it may be possible to satisfy (II.6) when the ϵ term is discarded. If $\epsilon > 0$, it can be discarded, and (II.6) then provides a sufficient condition, easily evaluated, in order that $\delta Q \geq 0$. On physical grounds, and according to the examples which have been calculated, the assumptions on which (II.5) and (II.6) are based, namely $\alpha > 0$ and $\beta \geq 0$, imply that $\delta\phi$ and hence δQ are greater than zero. This means that inequality (II.6) rather than (II.5) should apply. Also, since $\Sigma_1 - \Sigma_3 > 0$, we have $\epsilon > 0$. In other words (II.5) will probably never be satisfied and the sufficient condition (II.6) may be satisfied. Similarly, if α and β are negative so that the flux is depressed in R_2 only one of the ensuing inequalities will in fact be applicable.

It is of some interest to compare the superposition approximation with the analytic solution in certain simple cases where the analytic solution may be obtained.



TWO SLAB WATER HOLES IN AN INFINITE REACTOR

(a) Two slab water holes in an infinite reactor

We first examine superposition for the case of two slab water holes, 4 cm thick, and 4 cm apart in an infinite reactor (see sketch on page 48). The correct flux, ϕ , and the superposition flux $\phi^{(s)}$, illustrated in Figure 9 (see page 50) are given respectively by the formulae:

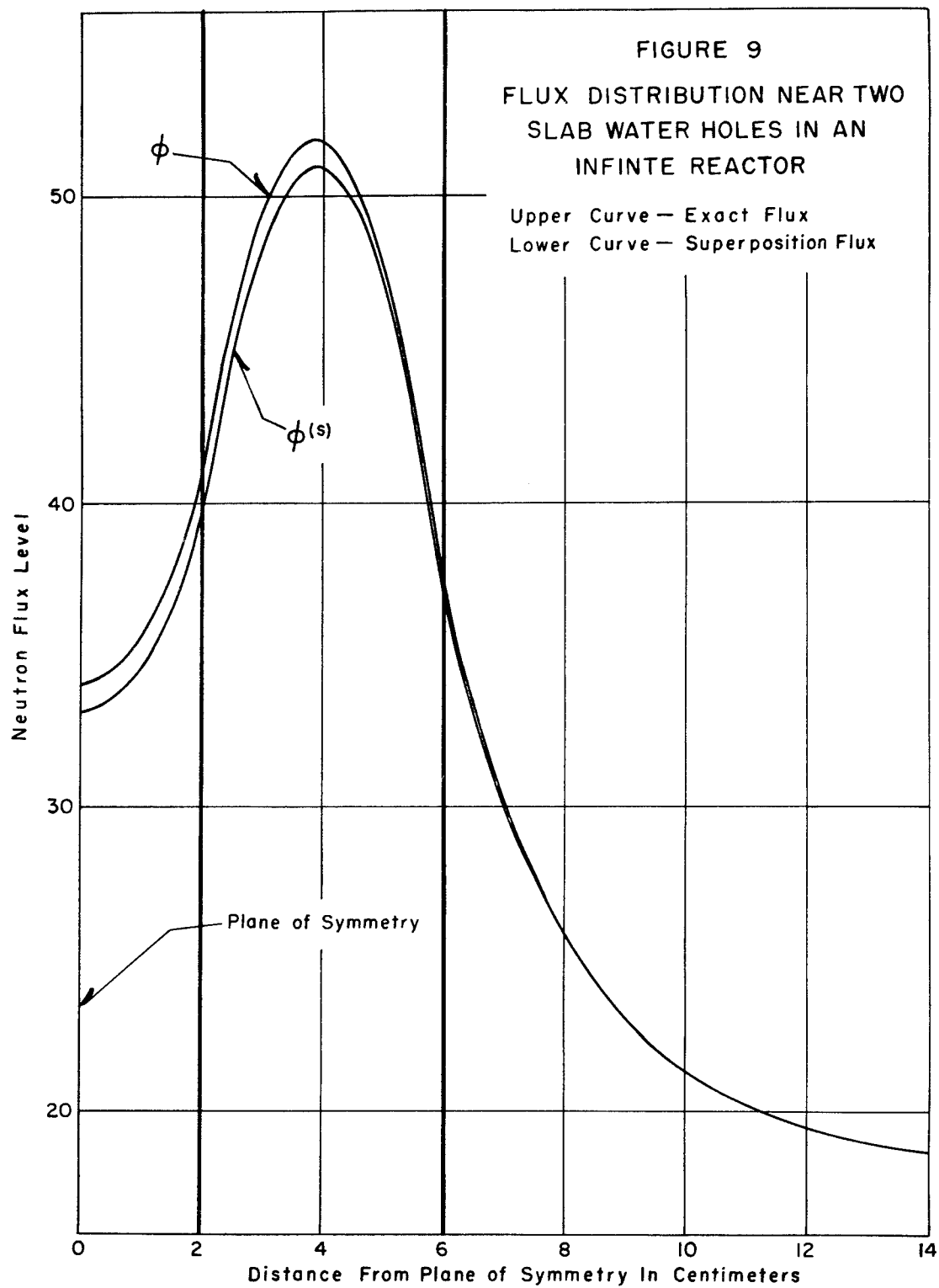
$$\begin{aligned}\phi &= 18.2 + 15.8 \cosh .447x, & 0 \leq x \leq 2 \\ &= 102.5 - 6.62 e^{.348x} - 97.1 e^{-.348x}, & 2 \leq x \leq 6 \\ &= 18.2 + 276.9 e^{-.447x}, & x \geq 6 \\ \phi^{(s)} &= 18.2 + 14.9 \cosh .447x & 0 \leq x \leq 2 \\ &= 102.5 - 52.8 \cosh \sqrt{.348}(x-4) + 44.6 e^{-.477(x+4)} & 2 \leq x \leq 6 \\ &= 18.2 + 274.0 e^{-.447x} & x \geq 6\end{aligned}$$

(b) The reflected slab reactor

We next examine superposition for a finite reflected slab reactor,^{*} Figure 10. The flux ϕ , the solution of $D\phi'' - \Sigma\phi + q = 0$, is given by the formulae

$$\begin{aligned}\phi &= c_1 \cosh \kappa_1 x + q_1/\Sigma_1, & x \text{ in } R_1 \\ &= c_2 e^{-\kappa_2 |x|} + q_2/\Sigma_2, & x \text{ in } R_2 \\ c_1 &= \frac{D_2 \kappa_2 (q_2/\Sigma_2 - q_1/\Sigma_1)}{D_2 \kappa_2 \cosh \kappa_1 a + D_1 \kappa_1 \sinh \kappa_1 a} \\ c_2 &= -c_1 (D_1 \kappa_1 / D_2 \kappa_2) e^{\kappa_2 a} \sinh \kappa_1 a.\end{aligned}$$

* This example was suggested by M. Danzker, Reactor Theory Section, Physics Department, Westinghouse Atomic Power Division



The superimposed flux, obtained by combining the fluxes when first one, then the other reflector is replaced by the reactor material, is given by:

$$\begin{aligned}\varphi^{(s)} &= 2d_1 e^{-\kappa_1 a} \cosh \kappa_1 x + q_1 / \Sigma_1, & x \text{ in } R_1 \\ &= d_1 e^{-\kappa_1(x+a)} + d_2 e^{-\kappa_2(x-a)} + q_2 / \Sigma_2, & x \text{ in } R_2\end{aligned}$$

with

$$\begin{aligned}d_1 &= \frac{D_2 \kappa_2 (q_2 / \Sigma_2 - q_1 / \Sigma_1)}{D_2 \kappa_2 + D_1 \kappa_1}, \\ d_2 &= \frac{D_1 \kappa_1 (q_2 / \Sigma_2 - q_1 / \Sigma_1)}{D_2 \kappa_2 + D_1 \kappa_1}.\end{aligned}$$

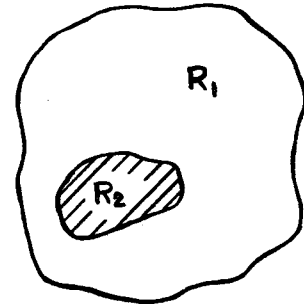
The ratio $(\varphi - \varphi^{(s)}) / (\varphi - q_1 / \Sigma_1)$ has been plotted in Figure 10, page 52, for several sets of values of the physical constants. In region R_1 this ratio is the constant,

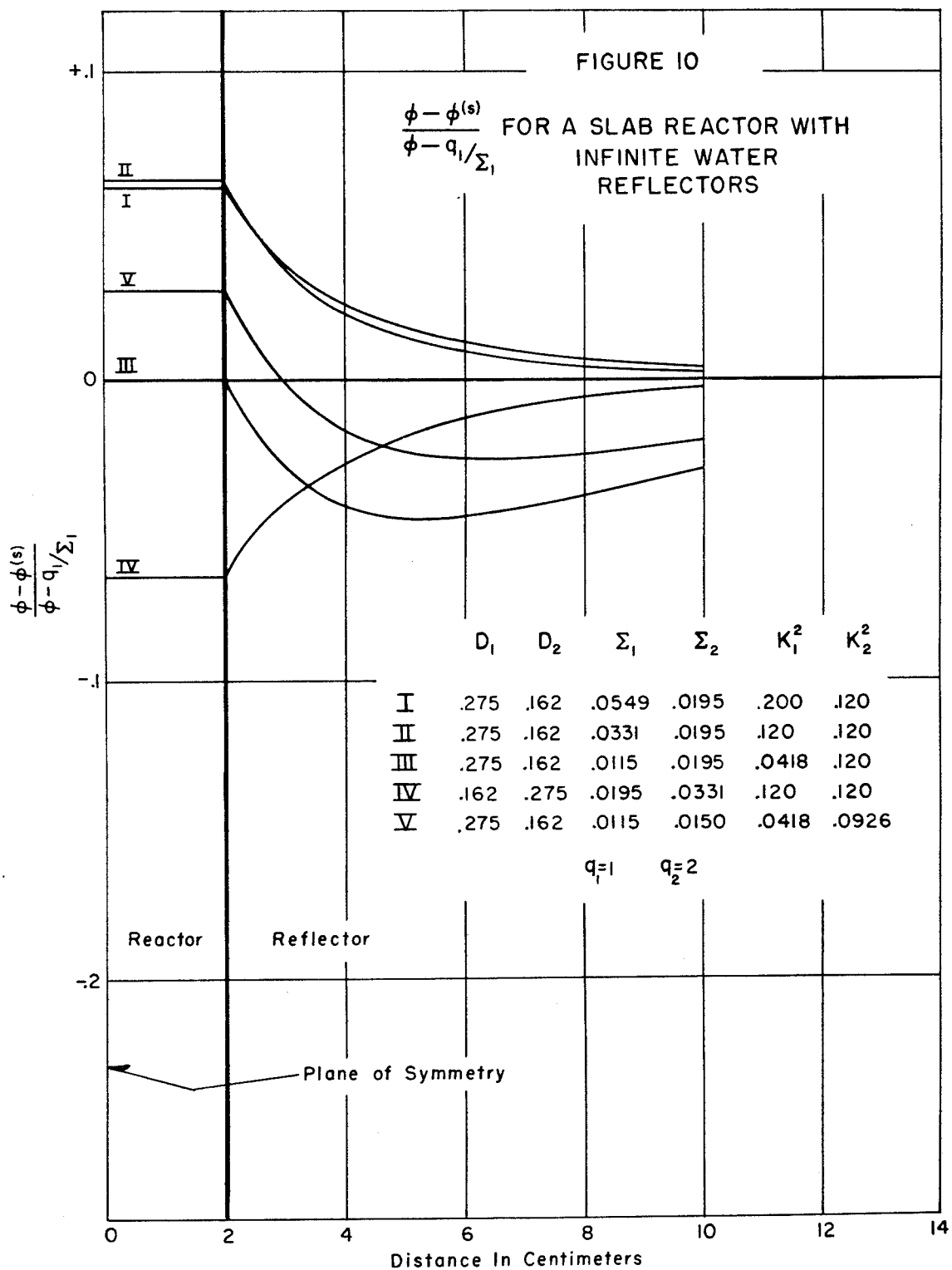
$$\frac{1 - (D_2 \kappa_2 / D_1 \kappa_1)}{1 + (D_2 \kappa_2 / D_1 \kappa_1)} e^{-2\kappa_1 a},$$

so that superposition gives the correct answer, underestimates or overestimates the flux in the core according as $D_2 \kappa_2 / D_1 \kappa_1 = 1$, < 1 , or > 1 . No simple relationship holds in the reflector. Indeed, as shown by curve V, Figure 10, $\varphi - \varphi^{(s)}$ can change sign.

2. Superposition by Multiplication

Consider a reactor of finite extent composed of two homogeneous parts, R_1 and R_2 . We have in mind a bare reactor with a water hole. The reflected reactor will be considered subsequently. Let φ_f be the assumed fast flux,





vanishing on the boundary and normalized so that $\max \varphi_f = 1$. The source terms are $q_2 = \Sigma_{f2}\varphi_f$ in R_2 and $q_1 = \Sigma_{f1}\varphi_f$ in R_1 (Σ_{f1} and Σ_{f2} are the fast, Σ_1 and Σ_2 the slow neutron absorption cross sections). Green's function G is the solution of $D_1 \nabla^2 G - \Sigma_1 G$ which vanishes on the boundary. The flux φ is the solution of the integral equation

$$D_i \varphi = (D_1 - D_2) \int_{S_2} \varphi \frac{\partial G}{\partial n} + (\kappa_1^2 - \kappa_2^2) D_2 \int_{R_2} G \varphi + \Sigma_{f1} \int_{R_1} \varphi_f G + \Sigma_{f2} \int_{R_2} \varphi_f G$$

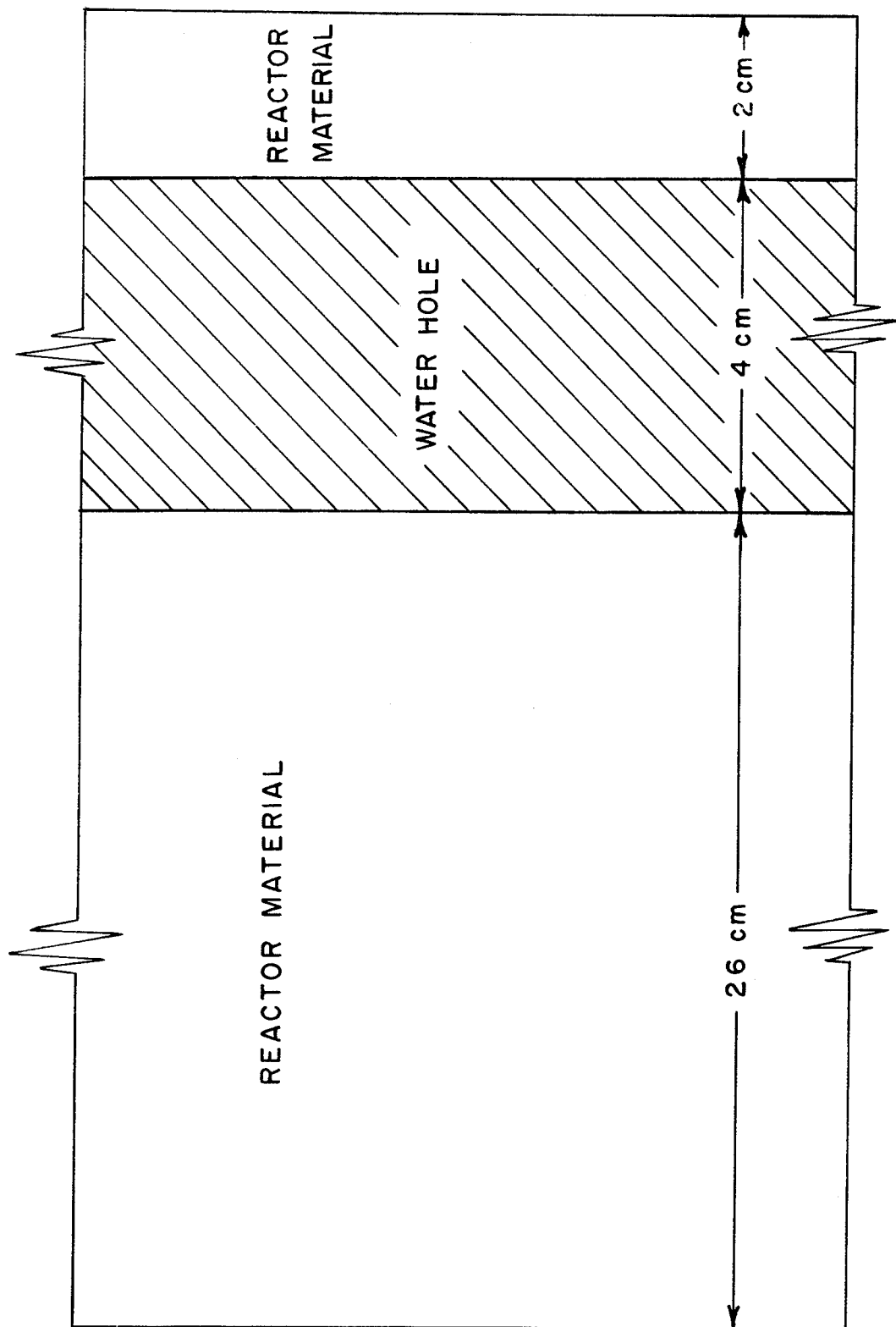
Now suppose the region R_1 extends to infinity and that the source terms are the constants Σ_{f1} and Σ_{f2} . Denote Green's function for this problem by G^* . The flux distribution, ψ , is the solution of

$$D_i \psi = (D_1 - D_2) \int_{S_2} \psi \frac{\partial G^*}{\partial n} + (\kappa_1^2 - \kappa_2^2) D_2 \int_{R_2} G^* \psi + \Sigma_{f1} \int_{\text{Space}} G^* + (\Sigma_{f2} - \Sigma_{f1}) \int_{R_2} G^*.$$

The superposed flux is $\varphi^{(s)} = \psi \varphi_f$; the error to be estimated is $\delta \varphi = \varphi - \psi \varphi_f$. Put $G^* = G + \delta G$. Then we can derive the following integral equation for $\delta \varphi$.

$$(II.7) \quad D_i \delta \varphi = (D_1 - D_2) \int_{S_2} \delta \varphi \frac{\partial G}{\partial n} + (\kappa_1^2 - \kappa_2^2) D_2 \int_{R_2} G \delta \varphi + \delta Q$$

$$(II.8) \quad \begin{aligned} \delta Q = & (D_1 - D_2) \left[\int_{S_2} \varphi_f \psi \frac{\partial G}{\partial n} - \varphi_f \int_{S_2} \psi \frac{\partial G}{\partial n} \right] + (\kappa_1^2 - \kappa_2^2) D_2 \left[\int_{R_2} \varphi_f \psi G - \varphi_f \int_{R_2} \psi G \right] \\ & + \Sigma_{f1} \left[\int_{R_1} \varphi_f G - \varphi_f \int_{R_1} G \right] + \Sigma_{f2} \left[\int_{R_2} \varphi_f G - \varphi_f \int_{R_2} G \right] \\ & - \varphi_f \left[(D_1 - D_2) \int_{S_2} \psi \frac{\partial \delta G}{\partial n} + (\kappa_1^2 - \kappa_2^2) D_2 \int_{R_2} \delta G \psi + \Sigma_{f1} \int_{R_1} \delta G + \Sigma_{f2} \int_{R_2} \delta G \right]. \end{aligned}$$



FINITE SLAB REACTOR WITH INTERNAL WATER REFLECTOR

As was to be expected, $\delta\phi$ satisfies an integral equation which differs from the equation satisfied by ϕ only in the inhomogeneous term δQ . Equation (II.8) furnishes justification for superposition by multiplication since δQ will be small provided R_1 is large enough for δG to be small, and provided ϕ_f does not vary rapidly over the regions which are significant in the integrations. Hence R_2 should not be too large nor too near the boundary of R_1 .

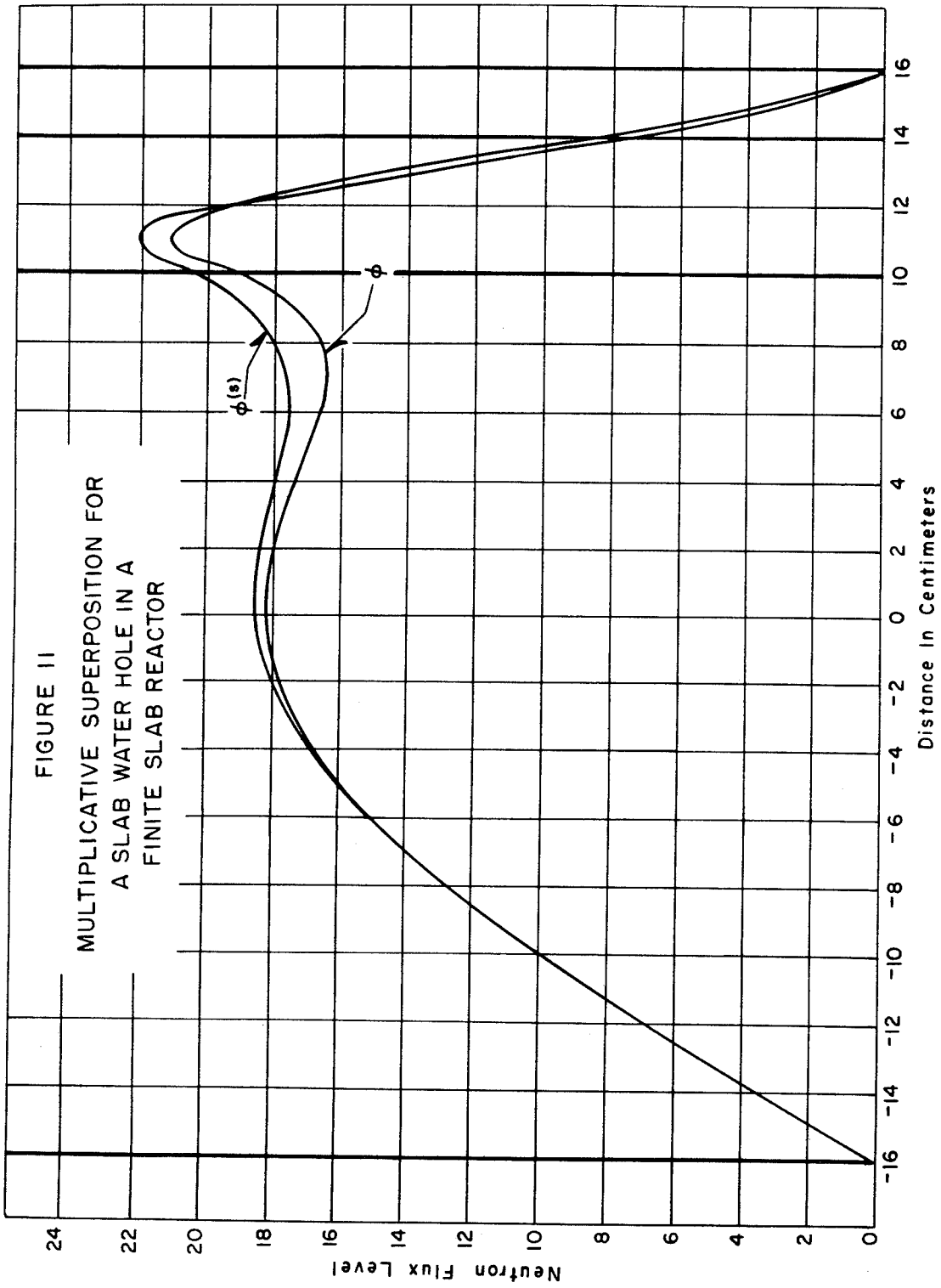
By way of illustrating what can be expected of multiplicative superposition, the flux pattern created by a slab water hole in a finite slab reactor having the STR constants has been examined exactly and by superposition. (See sketch on page 54.)

We are concerned here with a comparatively wide water hole very close to the boundary of the reactor. Using the STR constants given on page 25, and putting $\phi_f = \cos \frac{\pi x}{32}$ the thermal flux is found to be

$$\begin{aligned}\phi &= 18.2 \cos \frac{\pi x}{32} - 6.32 \times 10^{-8} e^{+.4471x} + .103 e^{-.4471x}, & -16 \leq x \leq 10, \\ &= 102.9 \cos \frac{\pi x}{32} - 120 e^{-.3471x} - .0218 e^{+.3471x}, & 10 \leq x \leq 14, \\ &= 18.2 \cos \frac{\pi x}{32} + 2766 e^{-.4471x} - 1.692 \times 10^{-3} e^{.4471x}, & 14 \leq x \leq 16.\end{aligned}$$

The superposition flux is

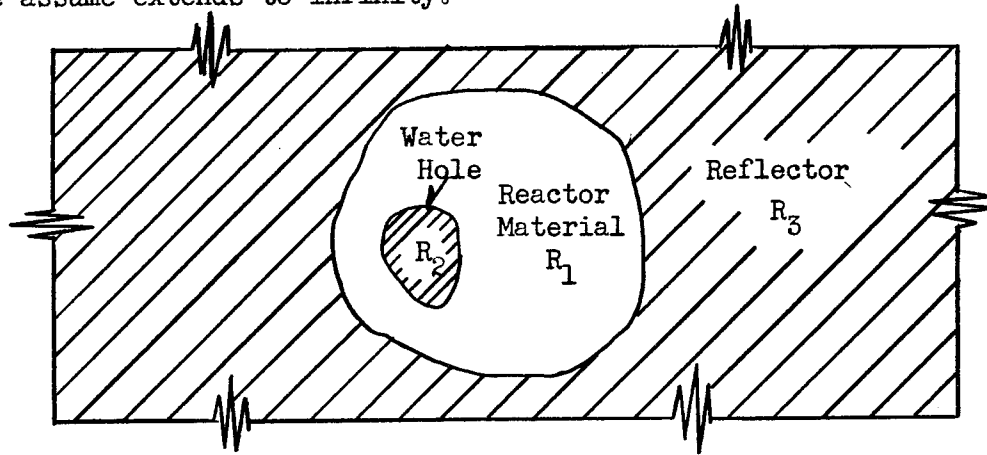
$$\begin{aligned}\phi &= \left\{ -53.3 \cosh[.347(x-12)] + 102.9 \right\} \cos \frac{\pi x}{32}, & 10 \leq x \leq 14, \\ &= \left\{ 44.8 e^{-.447(x-12)} + 18.2 \right\} \cos \frac{\pi x}{32}, & \begin{array}{l} -16 \leq x \leq 10 \\ 14 \leq x \leq 16. \end{array}\end{aligned}$$



The flux patterns are illustrated in Figure 11, page 56. Evidently the method of superposition provides a reasonable approximation to the correct flux.

3. Combined Superposition

Now let us look at a three region problem. Region R_1 is the reactor core, R_2 is, for example, a water hole inside the core, and R_3 is a reflector which we assume extends to infinity.



A method of approximating the flux distribution, ϕ , consists of multiplying that flux distribution, ψ , corresponding to a constant fast flux, by an appropriate weighting factor, ϕ_f . The flux distribution, ψ , corresponding to a constant fast flux, can in turn be approximated by superposing the flux patterns caused by R_2 and R_3 separately.

The flux ϕ is the solution of (II.1) with $q_i = \sum_{f,i} \phi_f$. The flux ψ satisfies the same integral equation with $q_i = \sum_{f,i}$. Then $\delta\phi = \phi - \psi\phi_f$ is the solution of

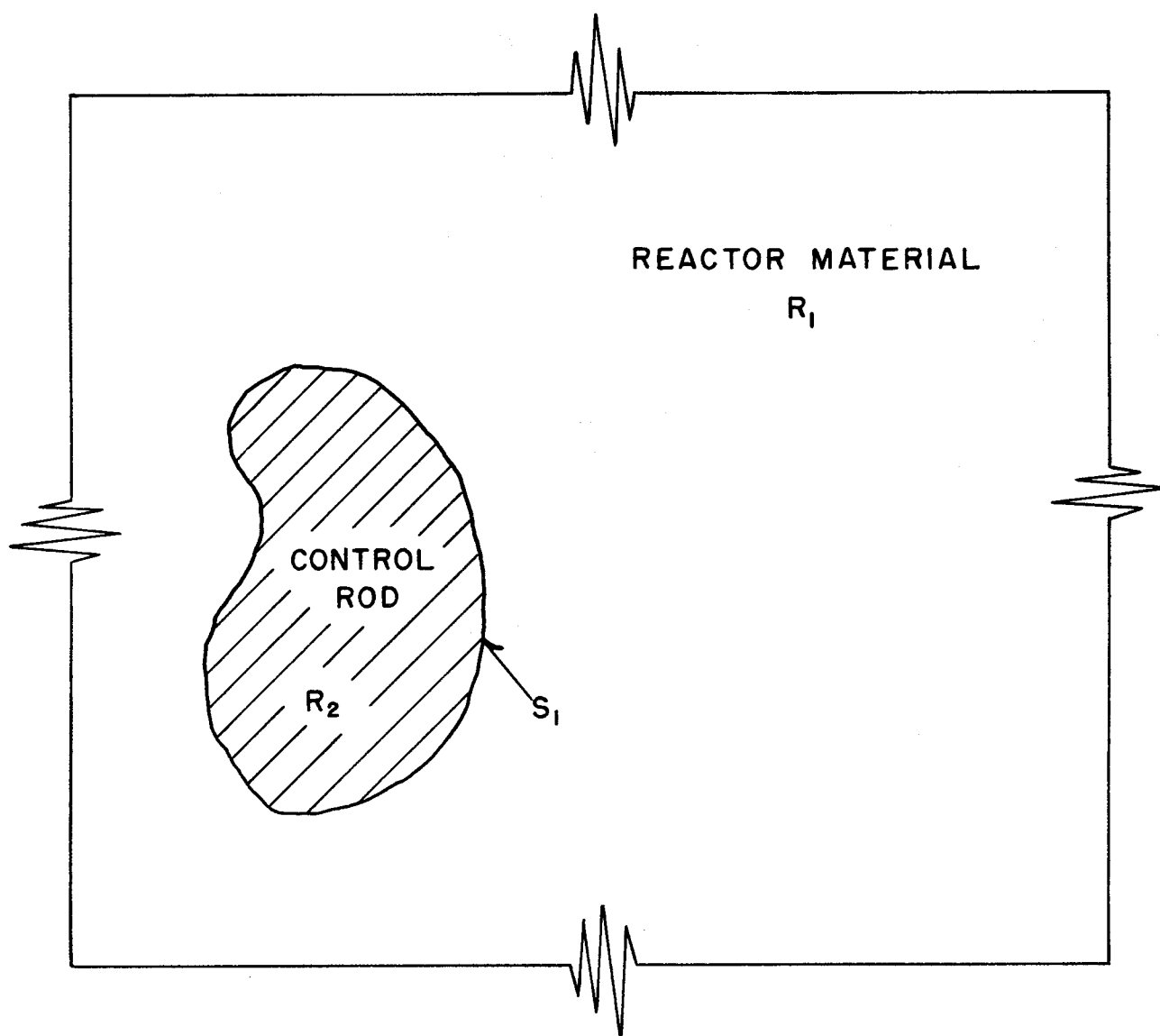
$$D_i \delta\phi = L(\delta\phi) + L(\psi\phi_f) - \phi_f L(\psi) + \int_{R_{1+2+3}} \sum_f \phi_f G - \phi_f \int_{R_{1+2+3}} \sum_f G \quad ;$$

and $\delta\phi$ will be small if ϕ_f does not vary too rapidly.

4. Conclusion

In retrospect it can be said that empirical evidence justifies the method of superposition under circumstances which at first sight seem drastic. In addition, there exist analytical expressions which provide a theoretical basis for superposition. On the other hand, attempts to estimate the superposition error by the formulae developed here would usually not be worth the effort.

If it is considered necessary to calculate the flux distribution in a complicated configuration more accurately than can be done by superposition, then it appears advantageous to solve the integral equation not for the flux φ , but for the error $\delta\varphi$ since this error is generally small and a slowly varying function. As was pointed out above, to a first approximation $D_i \delta\varphi = \delta Q$, a known function.



III. OTHER APPLICATIONS

In section 1 of part III we shall discuss the application of integral equations to control rods, and examine the superposition principle for control rods and for a control rod and a diffusing region. The extension of the integral equation method to multigroup and characteristic value problems will be outlined in section 2. Other aspects of the integral equations--perturbation formulae, variational principles, etc.,--will not be discussed in this report. These matters are not difficult although the presence of surface integrals differentiates the integral equations from those commonly treated in textbooks.

1. Control Rods

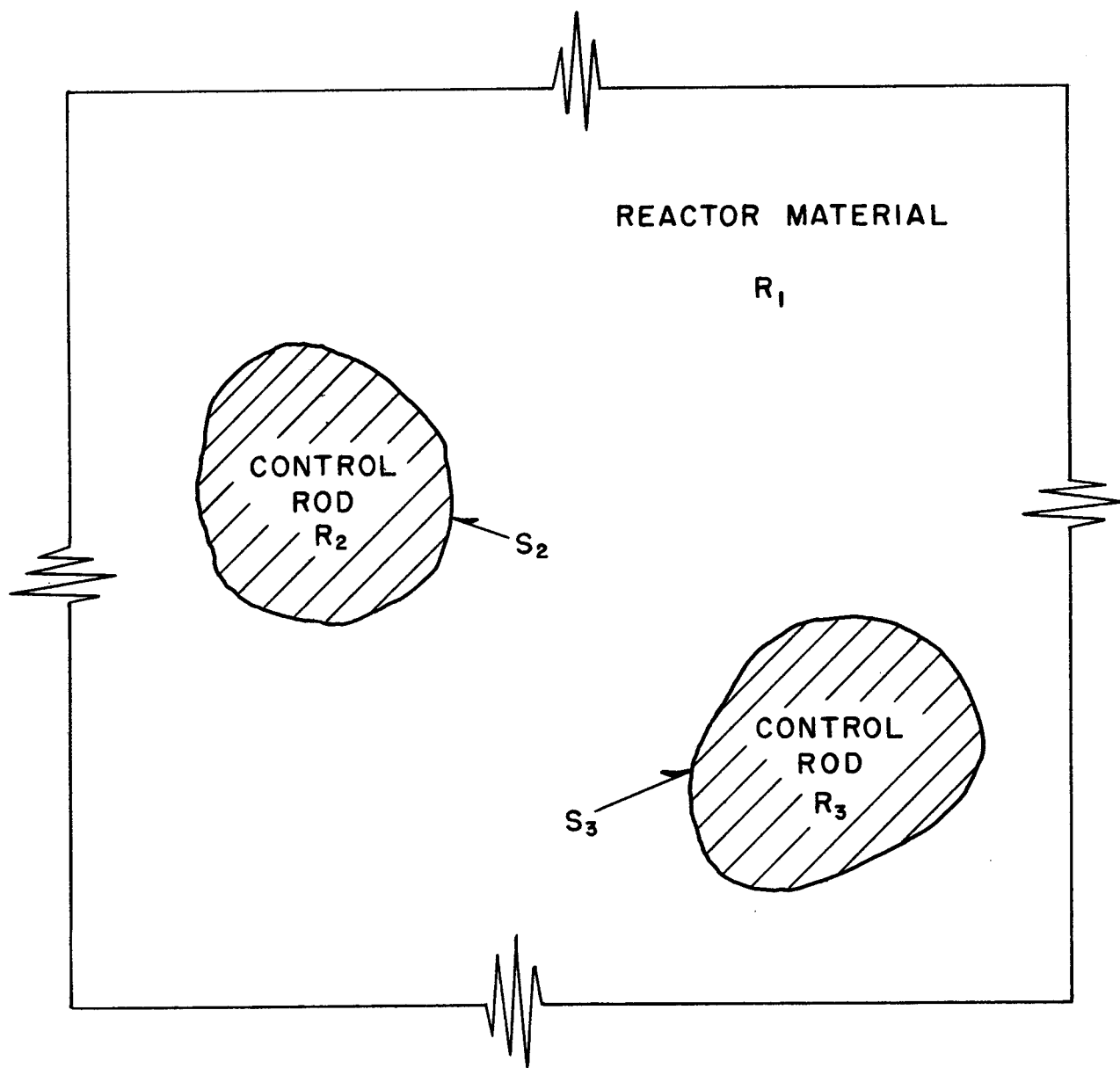
The integral equation ^{*} defining the flux in the neighborhood of a control rod is easily derived. Region R_2 in the sketch on page 59 is the control rod, R_1 is the diffusing medium. From the equations

$$\begin{aligned} D \nabla^2 \phi - \Sigma \phi + q &= 0 \\ D \nabla^2 G - \Sigma G &= 0 \end{aligned}$$

is derived the integral equation

$$\phi = - \int_{S_1} \left[\phi \frac{\partial G}{\partial n} - G \frac{\partial \phi}{\partial n} \right] + \int_{R_1} G \frac{q}{D} \quad .$$

* The integral equation (III.1) has been previously derived by M. Danzker of the Physics Department, Westinghouse Atomic Power Division.



The usual boundary condition is a relation between φ and its normal derivative:

$$\frac{\partial \varphi}{\partial n} = -\frac{\varphi}{\lambda},$$

where λ is a function of position on the surface S_1 . With this boundary condition the equation takes its final form:

$$(III.1) \quad \varphi = - \int_{S_1} \left(\frac{\partial G}{\partial n} + \frac{G}{\lambda} \right) \varphi - \int_{R_2} G \frac{q}{D} + \int_{R_{1+2}} G \frac{q}{D}.$$

A detailed discussion of equation (III.1) is unnecessary. We point out only that the integral equation can first be solved for the flux on the surface and then the flux elsewhere is obtained by integration.

2. Superposition of Control Rods

The integral equation satisfied by the flux distribution around two control rods in an infinite reactor (see sketch on page 61) can be written

$$\varphi = - \int_{S_{2+3}} \left(\frac{\partial G}{\partial n} + \frac{G}{\lambda} \right) \varphi - \int_{R_{2+3}} G \frac{q}{D} + \int_{R_{1+2+3}} G \frac{q}{D}.$$

The flux patterns $\varphi^{(2)}$ and $\varphi^{(3)}$, created by the rods R_2 and R_3 separately, satisfy the equations

$$\varphi^{(i)} = - \int_{S_i} \left(\frac{\partial G}{\partial n} + \frac{G}{\lambda} \right) \varphi^{(i)} - \int_{R_i} G \frac{q}{D} + \int_{R_{1+2+3}} G \frac{q}{D}, \quad i = 1, 2.$$

The superposed flux is defined to be $\varphi^{(s)} = \varphi^{(1)} + \varphi^{(2)} - q/\Sigma$. Hence the error $\delta \varphi = \varphi - \varphi^{(s)}$ is the solution of

$$\delta \varphi = - \int_{S_{2+3}} \left(\frac{\partial G}{\partial n} + \frac{G}{\lambda} \right) \delta \varphi - \int_{S_2} \left(\frac{\partial G}{\partial n} + \frac{G}{\lambda} \right) \left[\varphi^{(3)} - \frac{q}{\Sigma} \right] - \int_{S_3} \left(\frac{\partial G}{\partial n} + \frac{G}{\lambda} \right) \left[\varphi^{(2)} - \frac{q}{\Sigma} \right].$$

As was the case when R_2 and R_3 are diffusing media, the error in superposition depends on the deviations of the individual flux patterns from their asymptotic values.

The last example we shall mention is the superposition of a control rod, R_3 , and a diffusing region, R_2 , in an infinite reactor, R_1 . The integral equations for φ and the superposition error $\delta \varphi$ are:

$$D_i \varphi = (D_1 - D_2) \int_{S_2} \varphi \frac{\partial G}{\partial n} + (\kappa_1^2 - \kappa_2^2) D_2 \int_{R_2} G \varphi - \int_{S_3} \left(\frac{\partial G}{\partial n} + \frac{G}{\lambda} \right) \varphi + \int_{R_1} q_1 G + \int_{R_2} q_2 G, \quad i = 1, 2.$$

$$D_i \delta \varphi = (D_1 - D_2) \int_{S_2} \delta \varphi \frac{\partial G}{\partial n} + (\kappa_1^2 - \kappa_2^2) D_2 \int_{R_2} G \delta \varphi - \int_{S_3} \left(\frac{\partial G}{\partial n} + \frac{G}{\lambda} \right) \delta \varphi + (D_1 - D_2) \int_{S_2} \left[\varphi^{(3)} - \frac{q_1}{\Sigma_1} \right] \frac{\partial G}{\partial n} + (\kappa_1^2 - \kappa_2^2) D_2 \int_{R_2} \left[\varphi^{(3)} - \frac{q_1}{\Sigma_1} \right] \frac{\partial G}{\partial n} - \int_{S_3} \left(\frac{\partial G}{\partial n} + \frac{G}{\lambda} \right) \left[\varphi^{(2)} - \frac{q_1}{\Sigma_1} \right].$$

3. Generalizations

The extension of the integral equations derived above to include several energy groups of neutrons or to characteristic value problems offers no difficulty. Corresponding to each energy group there is an integral equation

whose source term is the source of neutrons appropriate to the group. For each group there will exist a Green's function which depends upon κ and the boundary conditions. Apart from questions of convergence, the characteristic value problem can be attacked by iteration since the ratios of successive iterates tend to a limit which determines the reactivity of the pile. For complicated geometries iteration of the integral equation or application of a variational principle provides perhaps the most useful approach. Of course the variational technique can be applied not only to the integral equations but to the multi-group differential equations as well. A disadvantage of the variational method is that not only do the fluxes have to be approximated but the adjoint fluxes also enter into the equations.